5 One-Dimensional Potential Steps, Barriers, and Wells

To familiarize ourselves with some of the most basic features of quantum systems, in this chapter we will apply the Schrödinger equation to simple, one-dimensional problems. Fortunately, it is possible to obtain qualitatively correct conclusions about the behavior of quantum particles in the presence of more or less arbitrary potentials by replacing these with piecewise-constant potentials, which significantly simplifies the mathematics. For example, for many purposes an attractive potential can be represented by a square potential well, and a repulsive potential by a square barrier (Fig. 5.1). Although real devices do not have perfectly discontinuous interfaces, the micro- and nanostructures that are manufactured today are modeled, to a very good approximation, by square potentials. Thus, for example, multilayer structures combining metal, vacuum and semiconductor materials have nearly discontinuous interfaces and can therefore be represented by square potential barriers, wells and steps.

Many modern nanoelectronic devices are designed to prevent electrons from moving in certain directions. A *quantum dot* confines electrons to a small volume, so it is called a zero-dimensional system. *Quantum wires*, such as nanotubes, are considered one-dimensional because they confine electrons to move in their two opposite directions. A *quantum well* is considered two-dimensional because it confines electrons to a plane. All of these structures today can be made of carbon atoms. The confinement starts when the dimension in the direction of the constraint is comparable to the de Broglie wavelength of the carrier, which can be of the order of a nanometer (10^{-9} m). Also the strong nuclear binding potential, which has a range of a few femtometers (10^{-15} m), can be represented, to a first approximation, by a finite square-well potential. As already mentioned, this replacement of the real potential by a simpler one that retains its basic characteristics has the great advantage of allowing us to study the essence of the physical situation using simple mathematical methods, as the following examples will illustrate.

5.1 General Approach

To deal with simple potential problems in the easiest and most transparent way, we will use the time-independent 1D Schrödinger equation

$$-\frac{\hbar^2}{2m}\psi'' + V\psi = E\psi, \tag{5.1}$$

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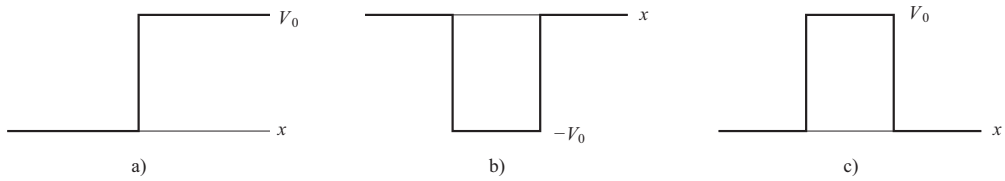


Figure 5.1 Piecewise constant potentials in one dimension. (a) The step potential, (b) The finite square well, (c) The square barrier.

which means that the solutions $\psi(x)$ will describe only stationary situations. This is an important restriction: it means that the system *has been given sufficient time to reach a stationary state*. With the introduction of the time-dependent Schrödinger equation in Chapter 7, a more complete and faithful description of quantum phenomena and their evolution in time will be possible.

Given that we will deal with potentials $V(x)$ that are piecewise constant, it is convenient to introduce two real parameters k and q, generally defined as

$$k^2 = \frac{2m}{\hbar^2}(E - V) \text{ when } E > V, \tag{5.2}$$

and

$$q^2 = \frac{2m}{\hbar^2}(V - E) \text{ when } E < V, \tag{5.3}$$

so that Eq. (5.1) is written as

$$\psi'' + k^2\psi = 0 \text{ when } E > V, \tag{5.4}$$

and

$$\psi'' - q^2\psi = 0 \text{ when } E < V. \tag{5.5}$$

Therefore, in those regions where $E > V$, the general solution will be of the form

$$\psi = Ae^{ikx} + Be^{-ikx}, \tag{5.6}$$

whereas in the regions where $E < V$, it will be of the form

$$\psi = Ce^{qx} + De^{-qx}, \tag{5.7}$$

with parameters A, B, C, D to be determined in each case by the conditions that must be satisfied for $\psi(x)$ and $\psi'(x)$ to be physical solutions. Specifically, we recall from Section 4.3 that ψ and ψ' must be finite, continuous, and single-valued functions at all points, in addition to satisfying the boundary conditions of the problem.

From Eqs. (5.6) and (5.7) it follows that the character of the solution depends drastically on whether the energy of the particles is greater or less than V: in the former case $\psi(x)$ is composed of oscillatory terms, with k^2 proportional to the (local mean) kinetic energy. From Eq. (4.83), we can identify the first term in Eq. (5.6) as representing the flow of particles to the right, with the velocity given by

$$v = \hbar k = \sqrt{2mE}, \tag{5.8}$$

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and the second term as representing the flow of particles to the left with the opposite velocity. In contrast, when $E < V$, ψ is the sum of exponentially increasing and decreasing terms at a rate given by q, with q^2 proportional to the energy deficit.

5.2 The Step Potential

We begin by considering the scattering of an ensemble of free particles (electrons, say) by the step potential shown in Fig. 5.1 (a). For convenience we place the discontinuity of V at $x = 0$. Although it is possible to treat the problem more generally by assuming that the particles approach the discontinuity from both sides, to simplify the analysis, we will consider that they hit the step only from the left. Further, we assume a stationary situation, where the beam intensity is constant and all particles travel with the same velocity and direction. We can then speak of a *monoenergetic* or *monochromatic* beam, the latter term meaning that a single de Broglie wavelength h/mv is assigned to all the particles in the beam, regardless of whether they are sent one by one or in bulk. Although this is an idealized situation, it allows us to obtain some physically meaningful results, as will be seen in what follows.

5.2.1 $E < V_0$, total reflection

In the region $x < 0$ the particles move with kinetic energy E, while in the region $x > 0$ this energy is not sufficient to compensate for the potential, so the $E - V_0$ difference becomes negative. Classically, this region is inaccessible to particles. The quantum situation is somewhat more complex, since from Eqs. (5.6) and (5.7) we have

$$\psi = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x \leq 0, \\ Ce^{-qx}, & x > 0. \end{cases} \tag{5.9}$$

with $k^2 = 2mE/\hbar^2$ and $q^2 = 2m(V_0 - E)/\hbar^2$, according to Eqs. (5.4) and (5.5). In the expression for $x > 0$ the term with positive exponential has been omitted, since it would make ψ increase indefinitely with x. For ψ and ψ' to be continuous at $x = 0$, it is required that $A + B = C; ik(A - B) = -qC$, whence

$$B = \frac{ik + q}{ik - q}A; \quad C = \frac{2ik}{ik - q}A, \tag{5.10}$$

which, when introduced in Eq. (5.9), gives

$$\psi = A\left[e^{ikx} + \frac{ik + q}{ik - q}e^{-ikx}\right], \quad x < 0, \tag{5.11}$$

$$\psi = \frac{2ik}{ik - q}Ae^{-qx}, \quad x > 0. \tag{5.12}$$

From the preceding expressions it follows that $|B| = |A|$. By writing $A = A_0e^{-i\alpha/2}$, $B = A_0e^{i\alpha/2}$ (which is a comfortable selection), with A_0 and α real, we obtain $C = A + B = 2A_0 \cos \alpha/2$. Therefore, from (5.9) we get

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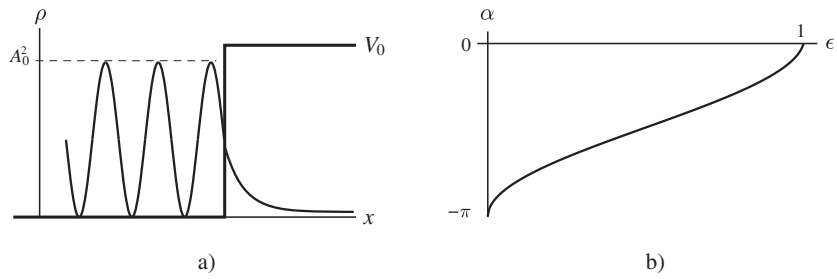


Figure 5.2 (a) Distribution of particles in the presence of a square potential step. (b) Phase shift α as a function of $\epsilon = E/V_0$.

$$\psi = 2A_0 \cos(kx - \alpha/2), \quad x < 0 \tag{5.13}$$

$$\psi = 2A_0 \cos(\alpha/2)\, e^{-qx}, \quad x > 0. \tag{5.14}$$

Since there is no net particle flow, we conclude that the number of particles reflected by the barrier is equal to the number of incident particles per unit time.

The particle density, given by the square of the expressions (5.13) and (5.14), is shown schematically in Fig. 5.2 (a). The effects of the interference of the concurring incident and reflected waves in the $x < 0$ region are clearly visible. The reflected wave is out of phase with the incident one by an amount

$$\alpha = \arccos\frac{k^2 - q^2}{k^2 + q^2} = \arccos(2\epsilon - 1) = -\arcsin 2\sqrt{\epsilon(1-\epsilon)}, \tag{5.15}$$

where $\epsilon = E/V_0$, $0 \le \epsilon \le 1$. Therefore, as $E \to 0$, $\alpha \to -\pi$, while as $E \to V_0$, $\alpha \to 0$; see Fig. 5.2 (b). It is interesting to compare these results with the optical case: we recall that when a light beam is reflected by a medium with lower refractive index there is no phase shift, while if the medium has a higher refractive index, the reflected wave is inverted with respect to the incident wave, that is, there is a phase shift of π. In the optical case, just as in the quantum case, at normal incidence (i.e., in 1D) the reflection from a mirror is total. In the $x > 0$ region, where there is no net particle transfer, one can speak of an *evanescent* solution, which decays exponentially with x according to Eq. (5.14).

This example serves to illustrate a remarkable phenomenon typical of QM. It is possible to change the phase shift α without changing the incident particle beam by altering the potential V_0 at $x = 0$; this modifies the distribution of particles in the entire region $x < 0$. From the point of view of the *description*, this is a nonlocal behavior, resulting from the interference of the two terms in the first of Eqs. (5.9). Other examples of such nonlocal behavior described by the wave function will be given in Section 4. The subject will be discussed in more detail in Sections 10.1.2 and 10.5.

5.2.2 $E > V_0$, partial transmission

In this case it is convenient to introduce the parameter k_1, defined as

$$k_1^2 = \frac{2m}{\hbar^2}(E - V_0), \tag{5.16}$$

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so that the general solution of the Schrödinger equation can be written as

$$\psi = Ae^{ikx} + Be^{-ikx}, \quad x < 0 \tag{5.17}$$

$$\psi = Ce^{ik_1 x} + De^{-ik_1 x}, \quad x > 0, \tag{5.18}$$

with $k_1 < k$. In the particular case we are analyzing, with the particles incident from the left, it is clear that the flow in the region $x > 0$ is exclusively to the right, so we must take $D = 0$. From the continuity conditions at $x = 0$ we get

$$B = \frac{k - k_1}{k + k_1} A, \quad C = \frac{2k}{k + k_1} A, \tag{5.19}$$

whence

$$\psi = A\left[e^{ikx} + \frac{k - k_1}{k + k_1} e^{-ikx}\right], \quad x < 0; \tag{5.20}$$

$$\psi = A\frac{2k}{k + k_1} e^{ik_1 x}, \quad x > 0. \tag{5.21}$$

Using this wave function, we can calculate the net flux of particles both to the left and to the right of the barrier. From Eq. (4.83) we obtain the following expression for the current density $j = \rho v$, for $x < 0$,

$$j_< = \frac{i\hbar}{2m}\left(\psi \frac{d\psi^*}{dx} - \psi^* \frac{d\psi}{dx}\right)\Bigg|_{x<0} = j_{\text{inc}} - j_{\text{refl}}, \tag{5.22}$$

where the incident and reflected current densities are given respectively by

$$j_{\text{inc}} = \frac{\hbar k}{m}|A|^2, \quad j_{\text{refl}} = \frac{\hbar k}{m}|B|^2. \tag{5.23}$$

Similarly, for $x > 0$ we obtain for the transmitted current density

$$j_> = j_{\text{trans}} = \frac{\hbar k_1}{m}|C|^2. \tag{5.24}$$

Since the boundary conditions guarantee that the flux density is continuous, both expressions (5.22) and (5.24) – whose value is constant – must be equal. It is not difficult to be convinced that the equality is in fact fulfilled by the values determined for B and C. Its physical meaning is clearly revealed by rewriting such an equality in the form

$$k|A|^2 = k|B|^2 + k_1|C|^2, \tag{5.25}$$

which says that the particles impinging on the barrier are either reflected or transmitted, so in this case there is partial reflection. This suggests introducing the *reflection coefficient* R and the *transmission coefficient* T, defined as follows,

$$R \equiv \frac{j_{\text{refl}}}{j_{\text{inc}}} = \frac{k|B|^2}{k|A|^2} = \frac{|B|^2}{|A|^2} = \left(\frac{k - k_1}{k + k_1}\right)^2, \tag{5.26}$$

$$T \equiv \frac{j_{\text{trans}}}{j_{\text{inc}}} = \frac{k_1|C|^2}{k|A|^2} = \frac{4kk_1}{(k + k_1)^2}. \tag{5.27}$$

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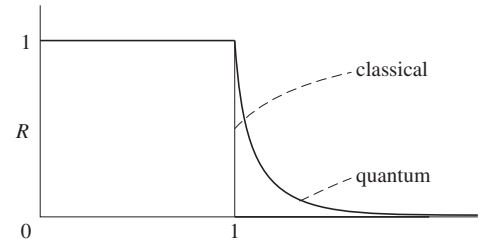


Figure 5.3 The reflection coefficient R as a function of $\epsilon = E/V_0$, for a beam of particles scattered by a square potential step.

It is clear that these coefficients satisfy the relation

$$R + T = 1, \tag{5.28}$$

which indicates that those particles that are not reflected are transmitted, that is, particles are neither lost nor created.

Figure 5.3 shows R as a function of $\epsilon = E/V_0$. As long as E is less than V_0 the reflection is total, $R = 1$, as we saw in the previous section. When $E > V_0$, particles can be transmitted according to Eq. (5.27), and they do so with increasing probability as E increases; when $E \gg V_0$, then $R \to 0$ and $T \to 1$, as expected. On the other hand, classical particles with $E > V_0$ would slow down, but all would be transmitted. This abrupt change of the reflection coefficient from 1 to 0 in the classical case is replaced by a continuous transition in the quantum case, as shown in Fig. 5.3.

It is easy to see that if we make the substitution $k \to -k_1$, $k_1 \to -k$, which corresponds to the case where the particle beam is sent from the right toward an attractive potential step, R and T are unchanged. Once again, the optical analogy is suggestive: according to a theorem of geometric optics, the transmission and reflection coefficients of a light beam passing through a medium with refractive index n_1 into a medium with index n_2 are equal to those obtained when the same beam passes from medium 2 into medium 1. Parameters like k, k_1, and so on, may therefore be considered as effective "refractive indices" – measured in suitable units – in the wave analog of QM.

Exercise E5.1. A two-dimensional barrier

Consider particles constrained to move in the xy-plane. The right half-plane $x > 0$ has the potential $V_0 > 0$, while the left half-plane $x < 0$ is held at zero potential. The particles can hit the boundary at $x = 0$ obliquely; the kinetic energy of the motion along the x-axis is $E_1 \leq V_0$, but that due to the motion along y is arbitrary. Determine the particle flux and analyze the results.

Solution. At the boundary there is total reflection in the x-direction, while the y-component travels freely. The wave function can be factorized in the form $\psi = \psi_1(x)\psi_2(y)$, where $\psi_2(y)$ is a plane wave with $E = E_2$ and $k = k_2$; $\psi_1(x)$ can be written as $\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$ for $x < 0$, and as $\psi_1(x) = Ce^{-qx}$ for $x > 0$, with $k_1^2 = 2mE_1/\hbar^2$ and $q = \sqrt{2m(V_0 - E_1)}/\hbar$. Therefore,

$$\psi_I(x, y) = (Ae^{ik_1x} + Be^{-ik_1x})e^{ik_2y}, \quad x < 0 \tag{5.29}$$

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$$\psi_{II}(x, y) = Ce^{-qx}e^{ik_2 y} \quad x > 0. \tag{5.30}$$

By stitching the solutions at $x = 0$, we get

$$\frac{B}{A} = \frac{k_1 - iq}{k_1 + iq} = e^{-2i\alpha}, \quad \frac{C}{A} = \frac{2k_1}{k_1 + iq} = 2e^{-i\alpha}\cos\alpha, \tag{5.31}$$

with

$$\tan\alpha = \frac{q}{k_1} = \sqrt{\frac{V_0}{E_1} - 1}. \tag{5.32}$$

Note that $|B| = |A|$, as would be expected from total reflection; this makes the current density along the x-axis equal to zero. In the y-direction we get

$$j_I = 2\frac{\hbar k_2}{m}|A|^2\,(1 + \cos 2(k_1 x + \alpha)) = \frac{\hbar k_2}{m}\rho_I(x), \tag{5.33}$$

$$j_{II} = 4\frac{\hbar k_2}{m}|A|^2 e^{-2qx}\cos^2\alpha = \frac{\hbar k_2}{m}\rho_{II}(x). \tag{5.34}$$

To the left of the barrier the incident wave and the reflected wave interfere, as shown by the oscillatory term. The current density in region II decays exponentially along the x-direction; this current vanishes when $\cos\alpha \to 0$, that is, $(V_0/E_1) \to \infty$. In electrodynamics, this condition would be equivalent to a perfect conductor, and the finite penetration for finite V_0 corresponds to the skin effect; the solution is usually called an evanescent wave, *although it carries no energy*.

Note that changing V_0 with k_1 and k_2 fixed only changes the phase of the interference pattern by modifying the relative phase between the incident and reflected waves. This shows the importance (and observability) of the relative phases, even though the global phase remains arbitrary.

5.3 The Square Well

We consider a square potential well like the one shown in Fig. 5.4, of width a and depth V_0, and divide the x-space into three regions I, II, and III, as in Chapter 4 (compare with Figure 4.6). To follow established conventions, we take the potential outside the well to be zero, so that a bound particle has negative energy, while particles with positive energy are scattered by the potential, but do not remain bound to it.

5.3.1 $-V_0 < E < 0$, bounded states

For negative energies, the particles are bound by the potential. In terms of the parameters

$$q^2 = -\frac{2mE}{\hbar^2} = \frac{2m}{\hbar^2}|E|, \tag{5.35}$$

$$k^2 = \frac{2m}{\hbar^2}\,(V_0 - |E|) \equiv \frac{2m}{\hbar^2}E', \tag{5.36}$$

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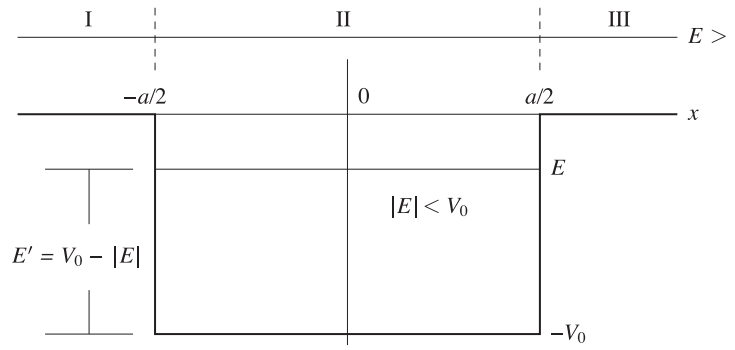


Figure 5.4 The finite-depth square well. For symmetry considerations, the origin of the x-coordinate is fixed at the center of the well.

the acceptable solutions of the Schrödinger equation are

$$\begin{aligned} \psi_I &= A_1 e^{qx}, && x < -a/2, \\ \psi_{II} &= B\cos kx + C\,\mathrm{sen}\,kx, && -a/2 < x < a/2, \\ \psi_{III} &= A_3 e^{-qx}, && x > a/2. \end{aligned} \tag{5.37}$$

When writing Eqs. (5.37) we have taken into account the requirement that ψ be bounded at every point. The solution inside the well has been written in terms of trigonometric functions (instead of imaginary exponentials), which have definite (odd or even) parity. Given that $V(x)$ is an even function of x, changing the sign of x will either keep the Schrödinger equation the same or change its sign; therefore the parity of ψ must be either even or odd. This means that there is a family of even solutions and a family of odd solutions, which are given respectively by

$$\psi_I = Ae^{qx}, \quad \psi_{II} = B\cos kx, \quad \psi_{III} = Ae^{-qx}, \qquad \psi(x) = \psi(-x), \tag{5.38}$$

$$\psi_I = Ae^{qx}, \quad \psi_{II} = C\sin kx, \quad \psi_{III} = -Ae^{-qx}, \qquad \psi(x) = -\psi(-x). \tag{5.39}$$

The conditions of continuity of ψ and ψ' at the boundaries $x = a/2$ and $x = -a/2$ give respectively

$$Ae^{-\frac{a}{2}q} = B\cos\tfrac{1}{2}ak, \quad qAe^{-\frac{a}{2}q} = kB\sin\tfrac{1}{2}ak, \qquad \psi(x) = \psi(-x), \tag{5.40}$$

$$Ae^{-\frac{a}{2}q} = -C\sin\tfrac{1}{2}ak, \quad qAe^{-\frac{a}{2}q} = kC\cos\tfrac{1}{2}ak, \qquad \psi(x) = -\psi(-x). \tag{5.41}$$

To simplify writing, we introduce the dimensionless variable $y = \frac{1}{2}ak$ and the parameter, also dimensionless, $y_0 = \frac{1}{2}\sqrt{2ma^2V_0/\hbar^2}$, so that

$$\tfrac{1}{2}aq = \sqrt{y_0^2 - y^2}. \tag{5.42}$$

5.3.1.1 Even and odd solutions

It is convenient to analyze each family separately. For even solutions, the first two equations (5.41) give

$$y\tan y = \sqrt{y_0^2 - y^2}. \tag{5.43}$$

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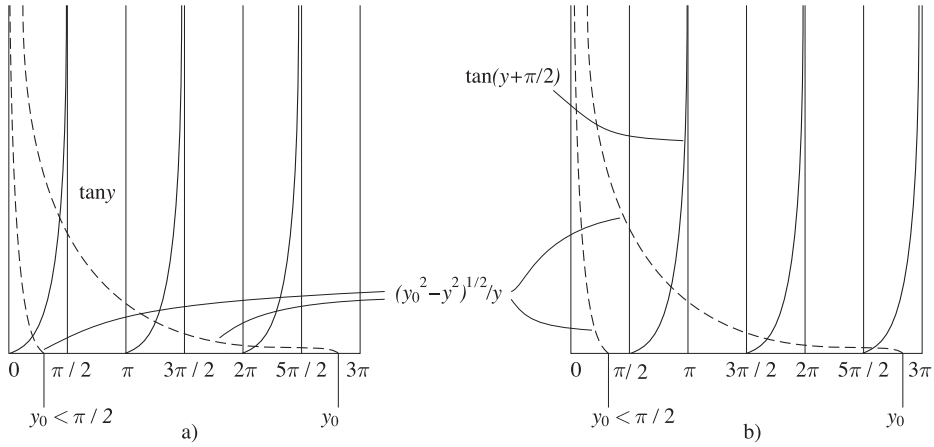


Figure 5.5 Solutions of the eigenvalue equation for the finite square well, for different values of the parameter y_0. (a) Even solutions, (b) odd solutions.

This is a transcendental equation, the solution of which can be obtained graphically from the intersections of the curves tan y and $\sqrt{y_0^2 - y^2}/y$, as shown in Fig. 5.5 (a). No matter how small the value of the parameter y_0, there exists at least one solution, meaning that a 1D well has at least one bounded state. In particular the ground-state solution is an even function. As y_0 grows, the number of intersections increases; that is, as the product $V_0 a^2$ increases, so does also the number of bounded states that the well can contain. In the limit where this product is infinite (the limit discussed in Section 4.3.6) the points of intersection become equidistant at the values $y = \pi/2, 3\pi/2, \ldots$ Therefore, for a potential well that is very deep or very wide or both, so that $y_0 \gg 1$, the energy eigenvalues are approximately given by the formula

$$y = \frac{a}{2\hbar}\sqrt{2mE'_n} = \pi\left(m + \tfrac{1}{2}\right), \tag{5.44}$$

where m is an integer and according to Eq. (5.36), E'_n is the energy measured from the bottom of the well. This expression, rewritten in the form

$$E'_n = \frac{\hbar^2\pi^2}{2ma^2}(2m+1)^2, \tag{5.45}$$

corresponds to the solutions of the infinite well with odd n, given by

$$E'_n = \frac{\hbar^2\pi^2}{2ma^2}n^2, \ n \text{ odd}. \tag{5.46}$$

The odd solutions are obtained following an analogous procedure; from the second pair of equations (5.41) the eigenvalue equation becomes

$$-y\cot y = \sqrt{y_0^2 - y^2}, \tag{5.47}$$

and its graphical solutions are shown in Fig. 5.5(b). We see that for $y_0 \to \infty$, the solutions correspond to $y = \pi, 2\pi, 3\pi, \ldots$, the values given by

$$E'_n = \frac{\hbar^2\pi^2}{2ma^2}n^2, \ n \text{ even}. \tag{5.48}$$

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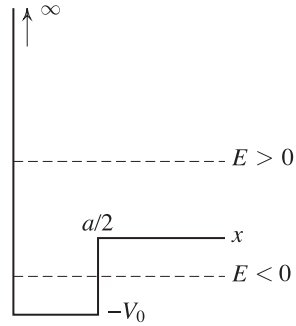


Figure 5.6 Effective square potential well of depth V_0 for central problems in two or three dimensions. The radius of the well is $a/2$.

If $y_0 < \pi/2$, there is no intersection, which means that for a 1D square well to have at least one odd bounded state, it is required that

$$a^2 V_0 > \frac{\pi^2 \hbar^2}{2m}. \tag{5.49}$$

Note that the odd solutions obtained here are also solutions of the potential shown in Fig. 5.6, since they cancel at $x = 0$ (precisely because they are odd), as required by the infinitely repulsive potential of this well at $x = 0$. As we shall see in Section 12.1, this is the type of effective potential for 2D and 3D central problems. From this we conclude that an attractive potential in two or three dimensions does not necessarily allow for bounded states; a condition of the type given by Eq. (5.49) must be satisfied for a first bounded state to occur.

In summary, we have shown that a 1D well always has bounded states that form a discrete spectrum; furthermore, the number of bounded states that fit in the well increases as a function of its effective width and depth.

Exercise E5.2. Quantum dots

A quantum dot can be thought of as electrons confined in a very small 3D box, a kind of artificial atom or zero-dimensional system. Find the eigenfunctions and eigenvalues for electrons found in an infinite 3D rectangular well and determine under what conditions the energy levels are degenerate.

Solution. Let a_1, a_2, a_3 be the x, y, z sides of the rectangular well. Solving Schrödinger's equation in a rectangular coordinate system, we obtain

$$\psi_{n_1 n_2 n_3} = \sqrt{\frac{8}{a_1 a_2 a_3}} \sin\left(\frac{\pi n_1}{a_1} x\right) \sin\left(\frac{\pi n_2}{a_2} y\right) \sin\left(\frac{\pi n_3}{a_3} z\right), \tag{5.50}$$

where the quantum numbers n_1, n_2, n_3 take any of the values $1, 2, 3, \ldots$ The total energy is given by

$$E_{n_1 n_2 n_3} = \frac{\pi^2 \hbar^2}{2m} \left(\frac{n_1^2}{a_1^2} + \frac{n_2^2}{a_2^2} + \frac{n_3^2}{a_3^2}\right). \tag{5.51}$$

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It is not difficult to see that if the relation between two sides is an integer $k, a_2 = ka_1$, then there is a degeneracy for the pair of quantum numbers n_1, n_2 whenever n_2/k is an integer. Indeed, if n_1 is replaced with n_2/k and n_2 with $n_1 k$, the same energy is obtained as for n_1 and n_2. In particular, if two sides of the well are equal, there is a degeneracy of order $g = 2$ whenever $n_1 \neq n_2$. It remains for the student to find the energy degeneracy as function of the quantum numbers when the well is cubic.

As quantum dots have very few electrons, their relative simplicity has allowed them to be used successfully for detailed theoretical-experimental studies of the effects of electron–electron interactions, transport effects, and so on. Applications of low-dimensional systems in the fabrication of solid-state devices are already numerous (e.g., very low-noise amplifiers for satellite and communication antennas) and will certainly develop further.

5.3.2 $E > 0$, resonant transmission and resonant scattering

For positive energies, the solutions are oscillatory in the three regions,

$$\begin{aligned} \psi_I &= A_1 e^{ikx} + B_1 e^{-ikx}, \quad x < -a/2 \\ \psi_{II} &= A_2 e^{ik_1 x} + B_2 e^{-ik_1 x}, \quad -a/2 < x < a/2 \\ \psi_{III} &= A_3 e^{ikx} + B_3 e^{-ikx}, \quad x > a/2, \end{aligned} \tag{5.52}$$

with

$$k^2 = \frac{2mE}{\hbar^2}, \quad k_1^2 = \frac{2m}{\hbar^2}(E + V_0). \tag{5.53}$$

We write the continuity conditions of ψ and ψ', taking into account that when the particles approach the well from the left, in the region $x > a/2$ there are only transmitted particles flowing to the right, i.e., once again we should take $B_3 = 0$. Thus,

$$A_1 e^{-\frac{ia}{2}k} + B_1 e^{\frac{ia}{2}k} = A_2 e^{-\frac{ia}{2}k_1} + B_2 e^{\frac{ia}{2}k_1} \tag{5.54}$$

$$A_2 e^{\frac{ia}{2}k_1} + B_2 e^{-\frac{ia}{2}k_1} = A_3 e^{\frac{ia}{2}k} \tag{5.55}$$

$$k\left[A_1 e^{-\frac{ia}{2}k} - B_1 e^{\frac{ia}{2}k}\right] = k_1\left[A_2 e^{-\frac{ia}{2}k_1} - B_2 e^{\frac{ia}{2}k_1}\right] \tag{5.56}$$

$$k_1\left[A_2 e^{\frac{ia}{2}k_1} - B_2 e^{-\frac{ia}{2}k_1}\right] = k A_3 e^{\frac{ia}{2}k}. \tag{5.57}$$

We are left with five free parameters, so the four equations plus the normalization condition – which in this case is determined by the amplitude of the incoming beam A_1 – are satisfied without imposing any condition on the energy, and the spectrum is continuous, as it should be, since we are free to choose the energy of the incident beam.

To determine the reflection and transmission coefficients we must obtain the value of the coefficients B_1 and A_3. The calculation is somewhat laborious, so it is not included here; however, using the preceding equations it is easy to check the following results, which are plotted in Fig. 5.7,

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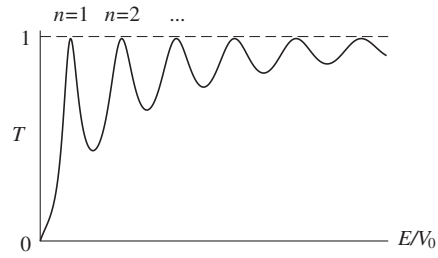


Figure 5.7 Transmission coefficient for free particles scattered by a square well, as a function of the ratio E/V_0.

$$R = \left|\frac{B_1}{A_1}\right|^2 = 1 - T; \tag{5.58}$$

$$T = \left|\frac{A_3}{A_1}\right|^2 = \left[1 + \frac{1}{4}\left(\frac{k_1}{k} - \frac{k}{k_1}\right)^2 \sin^2 k_1 a\right]^{-1}. \tag{5.59}$$

If $E \to \infty$, $k_1/k \to 1$, $(k_1/k) - (k/k_1) \to 0$ and $T \to 1$, as could be expected. However, also for $\sin k_1 a = 0$, i.e., for energy values such that

$$E + V_0 = \frac{\pi^2 \hbar^2}{2ma^2} n^2 \tag{5.60}$$

with integer n, the transmission coefficient takes the value $T = 1$. At exactly these energies all particles are transmitted (as would happen in the classical case for any positive energy). Here we have a 1D example of the phenomenon of *resonant transmission*, which will be discussed below and in more detail in Section 18.5.

The result just obtained can serve as a rudimentary model to explain phenomena such as the *Ramsauer–Townsend effect*.[1] This effect is observed in the scattering of low-energy electrons (< 1 eV) by noble gases, when at certain well-defined bombardment energies the electrons pass through the gas without being scattered. For example, argon is essentially transparent to electrons with energy 0.4 eV, but strongly scatters electrons with energy above or below this value. In wave language, we can explain such resonant transmission as being due to constructive interference between the left and right waves crossing the well, generated by multiple reflections at the discontinuities. Indeed, the maxima occur when the distance $2a$ travelled by the waves on their round trip is equal to an integer number of de Broglie wavelengths, as is clear from writing the expression $k_1 a = \pi n$ in the alternative form

$$\lambda = \frac{2\pi}{k_1} = \frac{2a}{n}. \tag{5.61}$$

Note that formula (5.60) agrees, except for the different convention on the origin of energy, with the expression (5.46) for the energy of the bounded states of the infinite well; for this reason, such levels are often called *virtual* energy levels.

Another interesting phenomenon exemplified by the previous results is that of resonances, or quasi-bounded states, which are so important, for example, in particle

[1] The effect is named after Carl Wilhelm Ramsauer (1879–1955) and Sir John Sealy Townsend, who independently studied the collisions between noble-gas atoms and low-energy electrons in 1921.

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theory. This occurs when the reflection coefficient takes a maximum value, which, as follows from Eqs. (5.58) and (5.59), occurs approximately at energy values such that

$$k_1 a = \left(n + \tfrac{1}{2}\right)\pi, \tag{5.62}$$

corresponding to the minima of the curve for T in Fig. 5.7. When this condition is met, we speak of a *resonance*. In this case the residence time turns out to be long and for this reason, such states are considered to be *quasi-bounded*.

5.3.3 Scattering matrix for one-dimensional problems

It is instructive, especially for future work, to consider the scattering problem from a more general perspective. For this purpose we introduce the important notion of *scattering matrix*, limited here to the 1D case. For an arbitrary potential vanishing at infinity on both sides, we can construct an incoming wave function in terms of the coefficients A_1 and B_3, as in Eqs. (5.52). It is convenient to represent the incident wave function as a column matrix,

$$\psi_{\text{inc}} = \begin{pmatrix} A_1 \\ B_3 \end{pmatrix}, \tag{5.63}$$

and similarly the outgoing wave function,

$$\psi_{\text{out}} = \begin{pmatrix} A_3 \\ B_1 \end{pmatrix}. \tag{5.64}$$

Note that at infinity, where $V(x) = 0$, the solutions of the Schrödinger equation are precisely the functions ψ_I and ψ_{III} in Eqs. (5.52), so knowledge of the incoming and outgoing matrices gives us the complete wave function in the asymptotic regions. Since the coefficients A_i and B_i are linearly related, see (5.54)–(5.57), we can establish a linear relationship between ψ_{inc} and ψ_{out} of the form

$$\psi_{\text{out}} = S\psi_{\text{inc}}, \tag{5.65}$$

where S is a 2×2 matrix. Explicitly, we shall write

$$\begin{pmatrix} A_3 \\ B_1 \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A_1 \\ B_3 \end{pmatrix} = \begin{pmatrix} S_{11}A_1 + S_{12}B_3 \\ S_{21}A_1 + S_{22}B_3 \end{pmatrix}. \tag{5.66}$$

The matrix S defined in this way, which transforms the incoming wave function into the outgoing one, is commonly called the *S-matrix* or *scattering matrix*. It can be shown that under the condition of conservation of flow, namely $T + R = 1$, the S-matrix is unitary, that is, it satisfies the condition $S^\dagger = S^{-1}$, or explicitly $S^*_{ij} = S^{-1}_{ji}$.

The S-matrix method provides a clear separation between the problem of determining the elements of S, which depend on the nature and dynamics of the system, and the initial conditions, which are arbitrary and depend on the specific problem. Thus, the study of the S matrix is equivalent to the general study of the system's dynamical behavior, independently of circumstantial or discretionary initial details. In the 1D case, the S-matrix allows us to determine the reflection and transmission coefficients, which contain the information about the properties of the scattering potential; the general 3D case is studied in Chapter 19.

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5.4 The Square Potential Barrier: Tunneling

The potential to be studied is a square repulsive barrier of width a and height V_0. As in the classical case, the solution depends drastically on whether the energy of the incident particles is higher or lower than the barrier potential. In the quantum case, however, the behavior of the beam has peculiar properties, as will be shown later.

5.4.1 $E < V_0$, the tunneling effect

As before, we consider only the case where the particles hit the barrier from the left. The problem is similar to the one studied in connection with the potential step in Section 5.2; however, its detailed study is interesting because in this case a new phenomenon arises, with important applications, namely the tunneling (or tunnel) effect. We will show that a fraction of particles – which can be appreciable – manages to pass the barrier and move freely on the other side of it. In the classical case this possibility is totally forbidden by the conservation of energy.

From Eqs. (5.6) and (5.7), the general solution in each of the three regions (with the barrier at $(0, a)$), is

$$\begin{array}{lll} I, x < 0: & \psi_I'' + k^2 \psi_I = 0, & \psi_I = A_1 e^{ikx} + B_1 e^{-ikx}, \\ II, 0 < x < a: & \psi_{II}'' - q^2 \psi_{II} = 0, & \psi_{II} = A_2 e^{qx} + B_2 e^{-qx}, \\ III, x > a: & \psi_{III}'' + k^2 \psi_{III} = 0, & \psi_{III} = A_3 e^{ik(x-a)} + B_3 e^{-ik(x-a)}. \end{array} \tag{5.67}$$

If particles are incident only from the left, $B_3 = 0$. Following the procedure used in the previous case, we obtain from the continuity conditions on ψ and ψ' that the coefficients can be written in the form

$$\begin{aligned} B_1 &= -i \frac{q^2 + k^2}{2kq} A_3 \sinh qa, \\ A_2 &= \frac{q + ik}{2q} A_3 e^{-qa}, \quad B_2 = \frac{q - ik}{2q} A_3 e^{qa}, \\ A_3 &= \frac{1}{\cosh qa + i \frac{1}{2} \left(\frac{q}{k} - \frac{k}{q} \right) \sinh qa} A_1, \end{aligned} \tag{5.68}$$

with the usual definitions for k and q. The transmission coefficient is given by $|A_3/A_1|^2$,

$$T = \left[1 + \tfrac{1}{4} \left(\frac{k}{q} + \frac{q}{k} \right)^2 \sinh^2 qa \right]^{-1}. \tag{5.69}$$

For $E = V_0$ we have $q = 0$, $\sinh qa = 0$, but $\lim_{q \to 0} \left(\frac{k}{q} + \frac{q}{k} \right)^2 \sinh^2 qa = k^2 a^2$, so that

$$T = \frac{1}{1 + \frac{1}{4} k^2 a^2} = \frac{1}{1 + \frac{m V_0 a^2}{2\hbar^2}} \quad (E = V_0). \tag{5.70}$$

As E decreases, so does T, but it is still nonzero, meaning that there is partial transmission of the beam through the barrier: this is the tunneling effect. Classically we should

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expect total, not partial, reflection of the incident beam, so tunneling is considered to be a quantum mechanical feature with no classical counterpart.

The transmission coefficient acquires its minimum value when E approaches 0 (hence $k \to 0$); for such small energies, if $qa \gg 1$, we can approximate the sinh with an exponential,

$$\sinh qa = \tfrac{1}{2}(e^{qa} - e^{-qa}) \approx \tfrac{1}{2}e^{qa} \quad (qa \gg 1), \tag{5.71}$$

and T reduces to

$$T = \left(\frac{4kq}{k^2 + q^2}\right)^2 e^{-2qa}. \tag{5.72}$$

The behavior of this function is dominated by the exponential, so we can approximate the preceding expression by

$$T \approx e^{-2qa} = \exp\left[-\frac{2a}{\hbar}\sqrt{2m(V_0 - E)}\right]. \tag{5.73}$$

Due to the critical dependence of T on qa, it is necessary to develop calculational techniques that allow us to deal with more realistic potentials. In Chapter 6 we will present a method that is especially useful in these cases. Suffice it to say that the tunneling effect is a widespread phenomenon that gives rise to spontaneous decay and is used both in laboratory applications (such as the tunneling microscope) and in technology (chips, transistors, tunnel diodes, etc.).

5.4.1.1 An intriguing phenomenon

The tunneling effect allows us to understand many aspects of conduction in metals and semiconductors, as well as other phenomena such as nuclear α decay, which will be discussed in Chapter 6. But the tunneling phenomenon itself is not well understood. The solution of Schrödinger's equation is usually taken as *the* explanation, and the name associated with it seems to obviate the need for further investigation. A word of caution, however: in reality, the particles do not simply tunnel through the barrier. Inside the barrier, p is imaginary, corresponding to an evanescent solution with no particle flow. So how is it that particles are transmitted and appear on the other side of the barrier, moving at the original speed?

It is difficult to explain the physical origin of the tunnel effect within the usual QM scheme, where the incident electrons are described by a function of energy that is the same for all electrons; the description in terms of fixed energy states does not take fluctuations into account. A plausible, more physically oriented explanation is offered by stochastic theories (see Chapter 10), which see QM as providing an excellent statistical, but not exhaustive description; the *fine* behavior of the electrons is lost in the coarse averaging. The transmission coefficient is an excellent, albeit indirect, measure of the probability of individual electrons crossing the barrier. An illustrative and explanatory set of detailed predictions using Nelson's stochastic version of QM (see Section 10.1) can be found in McClendon and Rabitz (1988).

Another point worth noting is that the wave function ψ_I, which describes the particles moving in region I, i.e., in front of the barrier, carries information about the width a and the height V_0 of the barrier. This is a nonlocality due to the stationary, statistical

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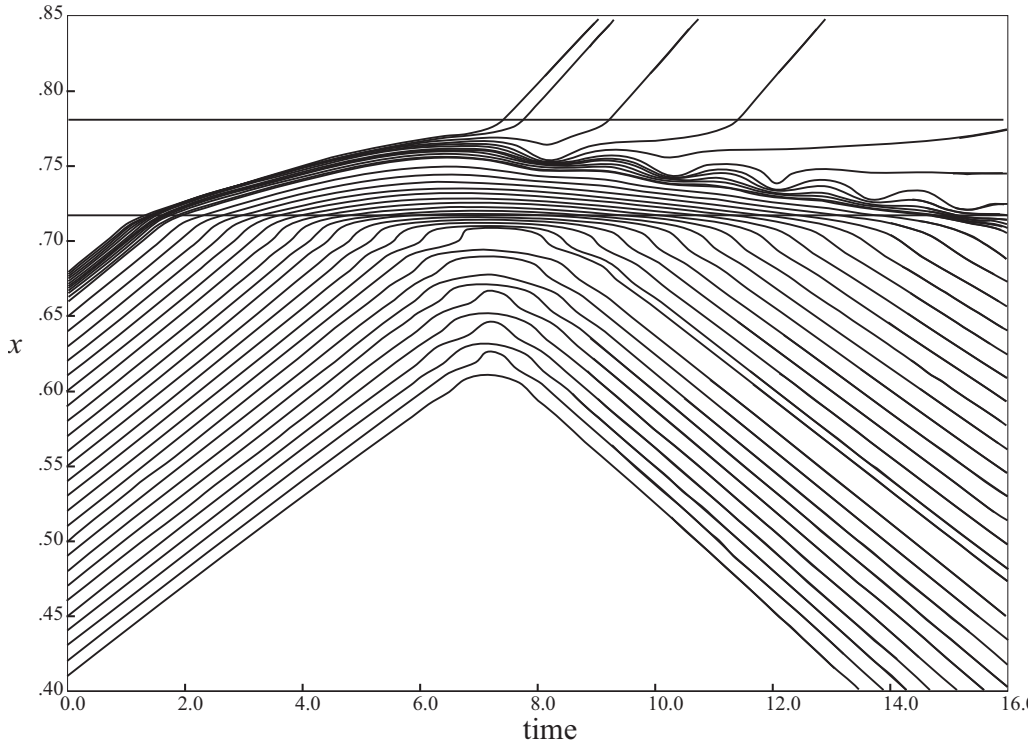


Figure 5.8 A collimated, monochromatic beam of particles scattered by a barrier, according to Bohm's theory (see Section 10.1). Note that many particles are scattered before reaching the barrier. Figure adapted from Dewdney and Hiley (1982).

description of the system. An impressive manifestation of this phenomenon is obtained by studying the trajectories of the particles (e.g., obtained from numerical simulations according to Bohm's theory, see Section 10.1.2), which clearly shows that a significant fraction of the incident particles are affected in their trajectory *before* they reach the barrier, as shown in Fig. 5.8.

5.4.1.2 Phase shift of the transmitted wave

It is instructive to analyze in more detail the transmitted wave $\psi_{\text{trans}} = \psi_{III}$. For this purpose we rewrite Eq. (5.68) as

$$\begin{aligned}\frac{A_3}{A_1} &= \frac{\cosh qa - i\frac{1}{2}\left(\frac{q}{k} - \frac{k}{q}\right)\sinh qa}{\cosh^2 qa + \frac{1}{4}\left(\frac{q}{k} - \frac{k}{q}\right)^2 \sinh^2 qa} \\ &= \frac{e^{i\delta}}{1 + \frac{1}{4}\left(\frac{q}{k} + \frac{k}{q}\right)^2 \sinh^2 qa} = \sqrt{T}e^{i\delta},\end{aligned} \tag{5.74}$$

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with the phase shift δ given by

$$\delta = \arctan \frac{1}{2}\left(\frac{q}{k} - \frac{k}{q}\right)\tanh qa. \tag{5.75}$$

Therefore, the transmitted wave is

$$\psi_{\text{trans}} = \sqrt{T}e^{ik(x-a)+i\delta}. \tag{5.76}$$

This result shows that the barrier produces two effects on the transmitted beam. The most evident one is the reduction of the wave amplitude, given by the factor $\sqrt{T}$; another effect is the phase factor $e^{i\delta}$ derived from the delay that the wave suffers when passing the barrier. In the limit where the barrier disappears we obtain $\delta = -\arctan ka \to 0$, which confirms that δ is effectively due to the presence of the barrier. (It is easier to go to this limit when $E > V_0$; then q becomes imaginary and $\tanh qa$ in Eq. (5.75) becomes $\tan qa$.) For this reason δ is called the *phase shift*. In Section 6.2.2 we return to this problem to determine the time delay produced by the barrier and in Section 18.4 it will be shown that particle scattering processes can be described in terms of these phase shifts.

5.4.1.3 Spontaneous decay

To gain some experience with the tunneling effect, we will use it as a basis for explaining the spontaneous decay of a system, for example, a radioactive nucleus. To do this, we modify the preceding potential by adding an infinitely rigid wall at $x = 0$, creating a well from which particles can only tunnel out to the right (Fig. 5.9). In this case the variable x represents the radial distance measured from the center of the well: the width of the well (i.e., its radius) is l and the width of the barrier is a. We write the solution of the Schrödinger equation as follows, taking A_1 real,

$$\begin{aligned}
\psi_I &= A_1 \sin kx, \\
\psi_{II} &= A_2 e^{-q(x-l)} + B_2 e^{q(x-l)}, \\
\psi_{III} &= A_3 e^{ik(x-l-a)} + B_3 e^{-ik(x-l-a)}.
\end{aligned} \tag{5.77}$$

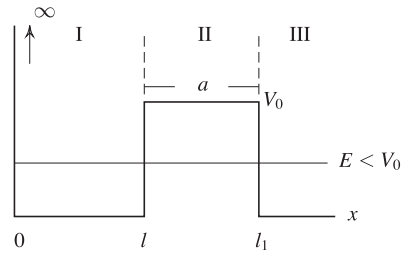


Figure 5.9 Schematic diagram of the potential well of width l, enclosed by a barrier of width a and height V_0, to show the phenomenon of spontaneous decay of a system as particles tunnel to the right. The number of particles inside the well decreases exponentially with time.

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As before, $k^2 = 2mE/\hbar^2$, $q^2 = 2m\,(V_0 - E)\,/\hbar^2$. After stitching together the solutions at the boundaries, we get

$$\begin{aligned}
A_2 &= \tfrac{1}{2}A_1\left(\sin kl - \frac{k}{q}\cos kl\right),\\
B_2 &= \tfrac{1}{2}A_1\left(\sin kl + \frac{k}{q}\cos kl\right),\\
A_3 &= \tfrac{1}{2}e^{-qa}\left(1 + \frac{iq}{k}\right)A_2 + \tfrac{1}{2}e^{qa}\left(1 - \frac{iq}{k}\right)B_2,\\
B_3 &= \tfrac{1}{2}e^{-qa}\left(1 - \frac{iq}{k}\right)A_2 + \tfrac{1}{2}e^{qa}\left(1 + \frac{iq}{k}\right)B_2.
\end{aligned} \tag{5.78}$$

These equations are satisfied for any energy $E < V_0$; therefore, the spectrum is continuous in principle. However, if we impose additional constraints, the spectrum can become discrete. In particular, this happens when the particles are initially confined in the well, so that in region III there are only particles escaping. In this case we must take $B_3 = 0$, from which it follows that

$$\left(\tan kl + \frac{k}{q}\right)\left[1 + \frac{k - iq}{k + iq}e^{-2qa}\right] = \frac{2k}{q}\frac{k - iq}{k + iq}e^{-2qa}. \tag{5.79}$$

This expression determines the discrete values for the energy of the quasi-confined particles. Comparing with Eq. (5.47), we see that the presence of a barrier of finite width modifies the energy levels of the particles inside the well; moreover, the solutions of Eq. (5.79) for k are complex, which implies a complex energy E. To see the meaning of this, we must refer to the complete expression for the wave function, including the exponential time factor, which is given by $\psi(x)e^{-iEt/\hbar}$. Therefore, the particle density inside the well is

$$\rho_I = |\psi_I e^{-\frac{iE}{\hbar}t}|^2 = |\psi_I|^2 e^{-\frac{i}{\hbar}(E - E^*)t} = |\psi_I|^2 e^{\frac{2\mathrm{Im}E}{\hbar}t}, \tag{5.80}$$

that is,

$$\rho_I = |\psi_I|^2 e^{-\lambda t}, \tag{5.81}$$

where the decay rate, λ, is given by

$$\lambda = -\frac{2}{\hbar}\mathrm{Im}E. \tag{5.82}$$

These equations show that the population inside the well decreases exponentially with time if the particles have complex energy ($\lambda \neq 0$), in other words, leakage through the barrier causes the population to decrease exponentially over time. The inverse of the parameter λ is the *mean* lifetime of the system, which means that over a period of time $t = 1/\lambda$ the population will decrease to the fraction $1/e \approx 35\%$ of its initial value. The reason this is called *spontaneous decay* is that there is no external factor causing the decay.

The conclusion is that the real part of the correction of k given by Eq. (5.79) with respect to the limit $a \to \infty$ (square well) represents a shift of the energy levels inside the well, while the imaginary part indicates that the states are no longer stationary and

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a decay takes place.[2] Note that while the population of region I decreases with time, that of region III must increase. In the present case the decay is due to the leakage of electrons trapped in the well; in the nuclear case, it will be the escape of α particles from a nucleus, and so on.

Exercise E5.3. Decay rate

Find an approximate formula to first order for the decay rate and its relationship to the transmission coefficient, assuming that the exact solution is close to the solution found for the infinitely wide barrier. Consider the case where the potential is large so that $ql \gg 1$, and the well is narrow so that $k_0 l \ll 1$.

Solution. To determine the decay (or escape) rate λ exactly, we would have to solve Eq. (5.79). We can solve it in an approximate way, considering that for an infinitely wide barrier ($a \to \infty$), the equation reduces to Eq. (5.47),

$$\tan kl + \frac{k}{q} = 0. \tag{5.83}$$

We write $E = E_0 + \delta E$, with E_0 the solution of this equation and δE the (complex) correction to the energy, and expand (5.79) in Taylor series around E_0. Since

$$k^2 = (k_0 + \delta k)^2 = \frac{2m}{\hbar^2} E = \frac{2m}{\hbar^2}(E_0 + \delta E), \tag{5.84}$$

the first-order terms give $2k_0 \delta k = (2m/\hbar^2)\delta E$, whence

$$k = k_0 + \delta k = k_0 + \frac{m}{\hbar^2 k_0}\delta E + \ldots, \tag{5.85}$$

Expanding (5.79) to first order in δk we obtain

$$\delta k(1 + ql \sec^2 k_0 l) = 2k_0 \frac{k_0 - iq}{k_0 + iq} e^{-2qa}. \tag{5.86}$$

If $k_0 l \ll 1$ (low energy, narrow well), we may take $\sec^2 k_0 l \simeq 1$. If, in addition, the potential is large so that for $ql \gg 1$, we can neglect unity against ql and write the above result in the form

$$\delta k = \frac{2k_0}{lq} \frac{k_0^2 - q^2 - 2ik_0 q}{k_0^2 + q^2} e^{-2qa}. \tag{5.87}$$

From this expression we obtain both the energy shift and the decay rate. In particular, using the relationship between the corrections to the wave number k and the energy E, we see that

$$\mathrm{Im}E \simeq \frac{\hbar^2 k_0}{m} \mathrm{Im}\delta k = -\frac{4\hbar^2 k_0}{ml} \frac{k_0^2}{k_0^2 + q^2} e^{-2qa}, \tag{5.88}$$

which when introduced in (5.82), gives

$$\lambda = \frac{8v}{l} \frac{k_0^2}{k_0^2 + q^2} e^{-2qa}, \tag{5.89}$$

[2] Note that by treating this problem as a stationary one, an inconsistency appears in the solution for ψ inside the well, due to the imaginary part of δk. To obtain the correct wave function one must solve the time-dependent Schrödinger equation, which is studied in Chapter 7.

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where $v = p/m = \hbar k_0/m$ stands for the velocity of the particles inside the well. Noting that in the preceding approximation, $q^2/(k_0^2 + q^2) \approx 1$, and using Eq. (5.72) for the transmission coefficient through the barrier, we write the preceding result in the form

$$\lambda = \frac{v}{2l} T. \tag{5.90}$$

This is the desired relationship between the decay rate and the transmission coefficient. The meaning of this formula can be understood by considering that $v/2l$ is the average number of times the particle hits the wall per unit time; this value multiplied by the probability T that the particle escapes each time gives the escape rate per unit time.

5.4.2 $E > V_0$, resonant transmission

This problem is analogous to those studied earlier. Although its algebra is somewhat more complicated, it leads to similar results and, in particular, to resonant transmission at energies defined by the condition $\sin qa = 1$, that is, for $qa = n\pi$. Specifically, the transmission and reflection coefficients are given by

$$T = 1 - R = \frac{1}{1 + \left[\frac{1}{4}\left(\frac{q}{k} + \frac{k}{q}\right)^2 - 1\right] \sin^2 qa}. \tag{5.91}$$

If q and k are very different, the resonance peaks can be very sharp and noticeable.

5.5 The Symmetric Double Well: Energy Splitting and Periodic Tunneling

The tunneling effect studied earlier shows that the stationary energy levels of a well are altered by the presence of neighboring potentials; in other words, the behavior of particles in a given region of space depends not only on the local potential in that region, but also on the potential that exists at every point in the available space. This is an important observation. For example, if we place another potential well next to the first, separated from it by a finite barrier, the introduction of the second well will modify the levels of the first, and vice versa.

Even more important than the level shift is the change in the number of possible stationary (or quasi-stationary, in the sense of the previous section) levels contained in each well. For example, we will see that in the case studied in this section, each level of one of the wells is split by the presence of the other well, producing a pair of closely spaced levels. This result reflects a general regularity: if a number of similar wells are placed side by side, separated by finite barriers, each original level will decompose into as many neighboring levels. In the next chapter we will see how this phenomenon allows us to understand in a simple way a number of properties of periodic structures, such as those of a crystal.

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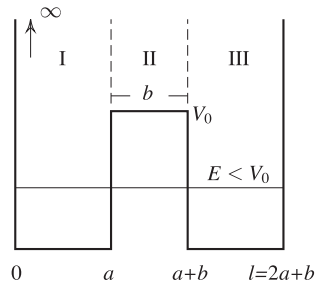


Figure 5.10 The symmetrical double well of total width $l = 2a + b$. Because the outer walls are impenetrable, there are stationary states inside.

Physically we can understand the phenomenon as follows. If we first imagine that each well is isolated by infinitely rigid walls and that the electrons are in a stationary state, then if we reduce the height of the barriers separating them, the boundary conditions of each well are modified, leading to an energy shift. Furthermore, the presence of an intermediate finite barrier allows particles to tunnel from one well to another, and the energy eigenvalues are consequently modified, as we saw in Section 4.

In the case of two wells separated by a finite barrier, as shown in Fig. 5.10, one well loses electrons by leakage and, on the other hand, it gains electrons that escaped from the second well. This double effect produces a level splitting. Clearly, the argument can be extended directly to the case of n similar wells. If the multi-well chain is bounded at both ends by infinitely repulsive potentials, as in Fig. 5.10, there are stationary states in the system, which occur when the flow of electrons escaping from one well is compensated by those entering from neighboring wells.

To find the energy levels of the double well we write the stationary solutions of the Schrödinger equation in the following form, limiting ourselves to the case $E < V_0$,

$$\begin{aligned} \psi_I &= A_1 \sin kx, \\ \psi_{II} &= A_2 e^{qx} + B_2 e^{-qx}, \\ \psi_{III} &= A_3 \sin k(l - x), \end{aligned} \tag{5.92}$$

with $l = 2a+b$. In writing Eqs. (5.92) the boundary conditions at $x = 0$ and $x = l$ have already been imposed. The remaining boundary conditions give the following relation between the constants,

$$\begin{aligned} A_1 \sin ka &= A_2 e^{qa} + B_2 e^{-qa}, \\ A_2 e^{q(a+b)} + B_2 e^{-q(a+b)} &= A_3 \sin ka, \\ kA_1 \cos ka &= q[A_2 e^{qa} - B_2 e^{-qa}], \\ q[A_2 e^{q(a+b)} - B_2 e^{-q(a+b)}] &= -kA_3 \cos ka. \end{aligned} \tag{5.93}$$

Since we have only three free constants to satisfy this system of four equations (one of them, A_1, for example, we fix by normalization), there is a condition between the parameters, which determines the allowed values for the energy E. To derive this quantization condition we first eliminate A_2 and B_2 from the previous system, thus obtaining the pair of equations

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$$A_1\left(\tan ka+\frac{k}{q}\right)=A_3\left(\tan ka-\frac{k}{q}\right)e^{-qb}, \tag{5.94}$$

$$A_1\left(\tan ka-\frac{k}{q}\right)=A_3\left(\tan ka+\frac{k}{q}\right)e^{qb}. \tag{5.95}$$

Dividing the first equation by the second gives the quantization condition

$$\left(\tan ka+\frac{k}{q}\right)^2=\left(\tan ka-\frac{k}{q}\right)^2 e^{-2qb}, \tag{5.96}$$

that is,

$$\tan ka+\frac{k}{q}=\pm\left(\tan ka-\frac{k}{q}\right)e^{-qb}. \tag{5.97}$$

Taking the limit $b\to\infty$ in this expression, we recover the quantization condition (5.47) for the potential well shown in Figure 5.6. Equation (5.97) confirms our expectations, since for finite b there is a correction with a double sign, that is, there are two possible values for ka. Therefore, if k_0 is a value of k corresponding to the well of Figure 5.6, the modified energies in the double well of Figure 5.10 are obtained by adding to k_0 the corrections calculated using (5.97). To estimate these first-order corrections, we take as a reference the value of k_0 given by (5.47),

$$\tan k_0a+\frac{k_0}{q_0}=0,\quad q_0=\frac{2m}{\hbar^2}V_0-k_0. \tag{5.98}$$

With $k=k_0+\delta k$ and expanding $\tan ka$ in Taylor series around k_0, we obtain (for $k_0a\ll 1$ and $q_0a\gg 1$)

$$\tan ka+\frac{k}{q}\approx\tan k_0a+a\delta k\sec^2 k_0a+\frac{k_0}{q_0}+\frac{\delta k}{q_0}\simeq a\delta k\left(1+\frac{1}{aq_0}\right)\simeq a\delta k \tag{5.99}$$

and

$$\tan ka-\frac{k}{q}\simeq\tan k_0a+\frac{k_0}{q_0}-\frac{2k_0}{q_0}=-\frac{2k_0}{q_0}. \tag{5.100}$$

Introducing these values into (5.97), we obtain to first order

$$\delta k\approx\mp\frac{2k_0}{aq_0}e^{-q_0b}. \tag{5.101}$$

It is left to the student to investigate the stationary wave functions for the lowest levels, both in the case of symmetric and antisymmetric solutions. In particular, it can be shown that the even wave function (with respect to the axis of symmetry of the potential) corresponds to the minimum energy of the system (with $\delta k<0$), while a slightly higher energy corresponds to the odd function (with $\delta k>0$). These two energies, denoted E_- and E_+, respectively, are given by the following expression, which follows directly from Eq. (5.101) and the definition of k, Eq. (5.6),

$$E_\pm=E_0\pm\delta E=E_0\pm\frac{4E_0}{aq_0}e^{-q_0b}. \tag{5.102}$$

The respective wave functions $\psi_\pm$ are shown schematically in Figure 5.11 (a).

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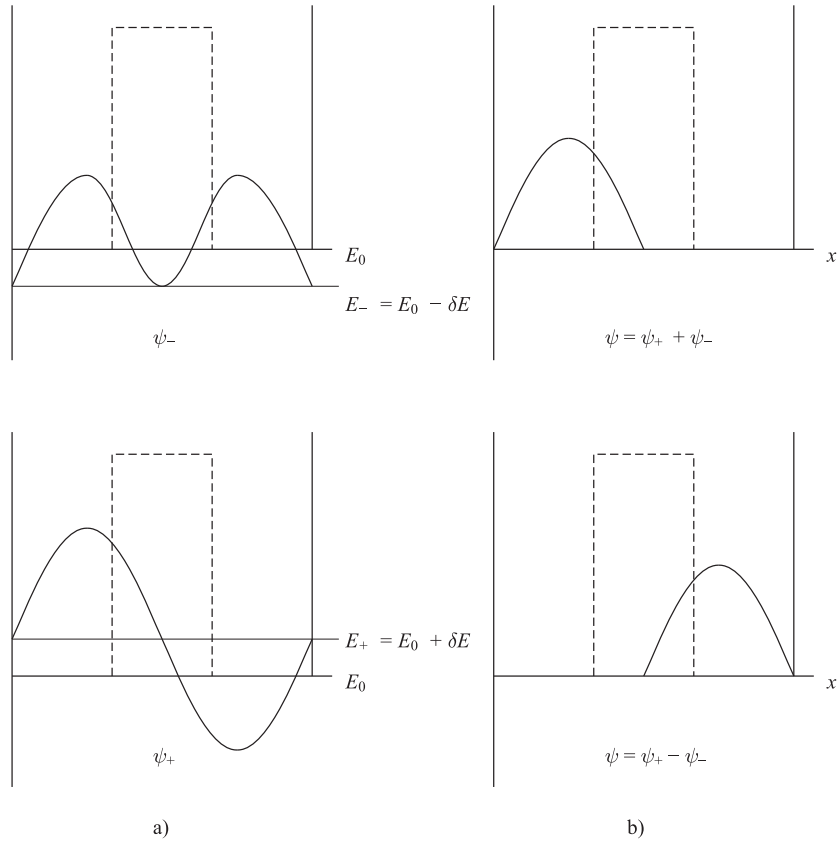


Figure 5.11 The symmetrical double well. (a) Symmetric and antisymmetric wave functions ψ_- and ψ_+ corresponding to the lowest energy levels, the first with a slightly lower energy than the second. (b) Distribution of particles in states $\psi_+ + \psi_-$ and $\psi_+ - \psi_-$.

5.5.1 Masers and molecular clocks

Suppose now that we use the stationary wave functions $\psi_\pm$ (which describe delocalized states, that is, with presence in both wells as shown in Figure 5.11a) to construct the following wave function (which is not an energy eigenfunction), by multiplying each (stationary) solution by its time factor,

$$\psi(x,t) = a\psi_+(x)e^{-\frac{iE_+}{\hbar}t} + b\psi_-(x)e^{-\frac{iE_-}{\hbar}t}. \tag{5.103}$$

We can select the coefficients a and b to satisfy any reasonable initial condition; in particular, for $t = 0$ we have

$$\psi(x,t=0) = a\psi_+ + b\psi_-. \tag{5.104}$$

As can be seen from Figure 5.11 (b), if $a = b$, the resulting wave function has a large maximum in the left well and is practically zero in the right well, that is, the particles are initially (almost) all located in the left well. With this initial condition, the wave function (5.103) becomes

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$$\psi(x,t) = a\left[\psi_+ e^{-\frac{i\delta E}{\hbar}t} + \psi_- e^{\frac{i\delta E}{\hbar}t}\right] e^{-\frac{iE_0}{\hbar}t} \tag{5.105}$$
$$= a e^{-\frac{iE_0}{\hbar}t}\left[(\psi_+ + \psi_-)\cos\frac{\delta E}{\hbar}t - i(\psi_+ - \psi_-)\sin\frac{\delta E}{\hbar}t\right].$$

At $t = 0$ the particles are indeed in the left well; but a time T later, given by $(\delta E/\hbar)T = \pi/2$, they will have migrated to the right well. Therefore, the wave function (5.105) represents a packet that periodically tunnels from one well to the other, with the period given by

$$2T = \frac{\pi\hbar}{\delta E} = \frac{\pi\hbar}{4E_0} a q_0 e^{q_0 b}. \tag{5.106}$$

It is possible not only to observe this effect, but to use it in the construction of technological devices. A typical example is provided by the ammonia molecule NH_3, which has a pyramidal structure with the three H atoms at the base and the N at the apex on either side of the plane defined by the three H atoms. Therefore, the intermolecular potential has a minimum at these two positions, that is, there are two wells separated by a barrier. For a qualitative analysis we can model this interatomic potential with rectangular wells. If we place ammonia in an electromagnetic field that oscillates with a period close to $2T$ (which corresponds to frequencies in the microwave band, with a wavelength close to 1.25 cm), the absorption of radiation by the molecule stimulates transitions between the two stationary states ψ_+, ψ_- separated by an energy $2\delta E$.

This phenomenon was exploited for the construction of the maser,[3] which essentially consists of a device containing NH_3 molecules initially in the ψ_+ state. When irradiated with the faint microwave field of frequency $\omega = 2\delta E/\hbar$ captured by a radio telescope, transitions to the ψ_- state are induced. The energy released is used to detect the presence of the radiation. The device functions as a microwave amplifier by stimulated emission of radiation, hence the name.

Clocks have also been built based on these transitions, to take advantage of the extraordinary stability of the operating frequency. Molecular clocks, which can be modelled as double potential wells, run with an accuracy of up to one second over several hundred years. This high precision made it possible to construct independent but synchronized clocks, which were used to verify some predictions of the theory of relativity to first order in v/c. In contrast, the usual interference experiments, which use a single clock and therefore require closed trajectories, only allow the observation of second-order effects, proportional to $(v/c)^2$.[4]

[3] Maser is an acronym for *microwave amplification by stimulated emission of radiation*. With further technological developments and the use of suitable transitions in other materials, light amplification by stimulated radiation was achieved, giving rise to the laser (see Section 17.2). These important devices act today both as amplifiers and generators. The initial work on masers was carried out independently in 1952–1954 by the Soviet physicists Nikolai Gennadievich Basov (1922–2001) and Alexandr Mijailovivh Prokhorov (1916–2002), and the American physicist Charles Hard Townes (1915–2015) and collaborators; all three were awarded the Nobel prize in 1964 for their contributions.

[4] In the 1990s, molecular clocks were replaced by atomic clocks, which can run to an accuracy of one second over 300 million years. This has led to the internationally agreed definition of the second based on the frequency of a particular transition of the caesium 133 atom, which is 9192631770 s^{-1}. Today, one of the most important applications of the amazing accuracy of atomic clocks is the GPS (Global Positioning System), used not only in telecommunications and transport, which was the original motivation, but also as a central element of mobile phones and other portable devices.

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5.6 Corollary: Meaning of Particle-Wave Behavior

Although all the problems considered in this chapter have involved the motion of particles subject to simple potential forces, the solutions obtained are reminiscent of the behavior of waves, such as string waves, water surface waves, sound waves or light waves. We have been forced to use the language of waves to describe the statistical behavior of particles. We talk about standing waves, or waves that travel in one direction or another, and we associate them with a wave number and a wavelength. We observe interference between these waves. Phase shifts and resonances occur here and there. In the tunneling effect the wave "penetrates" the barrier, just as an evanescent "wave" does in the optical case. And yet the particles represented by these waves never cease to be particles.

It is important to remember that just as the particles always retain their individuality and smallness, the statistics of the ensemble also retain their distributed properties. We see corpuscular behavior when attention is focused on the particle, and when attention is focused on the ensemble – the pattern traced by the large collection of particles – we may recognize what we think of as a wave. And indeed, it is the wave-like distribution just predicted by Schrödinger's "wave" equation. We are then in the presence of a most subtle stratagem of nature – as if it were "determined" to confuse us. In Chapter 10, we will come back to this topic and discuss it in the context of stochastic electrodynamics.

Problems

P5.1 A particle moves in a symmetric potential $V(x) = V(-x)$, such that the spectrum is discrete for $E < 0$ and continuous for $E > 0$. Draw a graph showing the general form of this potential if it is known that

(a) there are an infinite number of bounded states,
(b) there are a small number of bounded states.

Explain your argument. What would happen if the potential were not symmetric?

P5.2 Show that the principle of invariance against time reversal implies that, for a given energy, the coefficients of transmission and reflection by a potential step are the same, whether the particles are incident from the right or from the left.

P5.3 Calculate the reflection coefficient for particles of mass m and energy $E < 0$, incident from the left on the complex potential step.

$$V(x) = \begin{cases} 0, & x \leq 0, \\ (1 + ia)\, V_0, & x > 0, \end{cases} \tag{5.107}$$

where a is real and $V_0 > 0$.

P5.4 Show that a 1D square well has exactly $n + 1$ even bounded states if

$$\frac{2\pi^2\hbar^2}{ma^2} n^2 \leq V_0 < \frac{2\pi^2\hbar^2}{ma^2}(n+1)^2 \tag{5.108}$$

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and $n+1$ odd bound states if

$$\frac{2\pi^2\hbar^2}{ma^2}\left(n+\tfrac{1}{2}\right)^2 \leq V_0 < \frac{2\pi^2\hbar^2}{ma^2}\left(n+\tfrac{3}{2}\right)^2. \tag{5.109}$$

P5.5 Show that an extremely narrow and deep attractive potential that can be represented as a Dirac delta, $V(x) \simeq -\delta(x)/a$, contains a single bounded state, and find the corresponding energy eigenvalue. *Hint:* solve the Schrödinger equation for $x \neq 0$ and note that ψ' is not continuous at $x = 0$.

P5.6 Extend the study of the finite rectangular well to the 3D case using Cartesian coordinates. Show that if the well is very deep, the results of Exercise 5.22 are recovered.

P5.7 Study the energy degeneracy as a function of the quantum numbers for a cubic potential well with impenetrable walls.

P5.8 Show that the S-matrix for particles through a 1D potential is unitary. Use the result to prove the following relations,

$$|S_{11}|^2 + |S_{12}|^2 = 1, \quad |S_{21}|^2 + |S_{22}|^2 = 1, \quad S_{11}S_{12}^* + S_{21}S_{22}^* = 0. \tag{5.110}$$

P5.9 Determine the general form of the elements S_{ij} of the S-matrix describing the dispersion of particles through a 1D square well with $E > 0$.

P5.10 Determine the scattering matrix for the potential $V(x) = -a\delta(x-b)$.

P5.11 Derive in detail the formula (5.91) for the transmission coefficient of particles through a rectangular barrier when $E > V_0$.

Bibliographical Notes

A detailed and excellent textbook in two volumes is Cohen-Tannoudji et al. (1977). Other excellent, advanced textbooks are Gasiorowicz (2003) and Davydov (2013).

For the evolution of a wave packet, see Goldberg et al. (1967).

The website https://commons.wikimedia.org/wiki/Category:Animations_of_quantum_tunneling provides a list of 12 links to different versions of animations of quantum tunneling. You might try making your own animations for the problems discussed in this chapter.

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