Chapter 11
Elementary Cases

11.1 Introduction

The time-independent Schrödinger equation is a linear, second-order equation with a coefficient that depends on position. An analytical solution can be found in a limited number of cases, typically, one-dimensional ones. This chapter illustrates some of these cases, starting from the step-like potential energy followed by the potential-energy barrier. In both of them, the coefficient of the Schrödinger equation is approximated with a piecewise-constant function. Despite their simplicity, the step and barrier potential profiles show that the quantum-mechanical treatment may lead to results that differ substantially from the classical ones: a finite probability of transmission may be found where the classical treatment would lead to a reflection only, or vice versa. The transmission and reflection coefficients are defined by considering a plane wave launched towards the step or barrier. It is shown that the definition of the two coefficients can be given also for a barrier of a general form, basing on the formal properties of the second-order linear equations in one dimension. Finally, the case of a finite well is tackled, showing that in the limit of an infinite depth of the well one recovers the results of the particle in a box illustrated in a preceding chapter.

11.2 Step-Like Potential Energy

Consider a one-dimensional, step-like potential energy as shown in Fig. 11.1, with $V = 0$ for $x < 0$ and $V = V_0 > 0$ for $x > 0$. From the general properties of the time-independent Schrödinger equation (Sect. 8.2.3) it follows $E \geq 0$. To proceed, it is convenient to consider the two cases $0 < E < V_0$ and $E > V_0$ separately.

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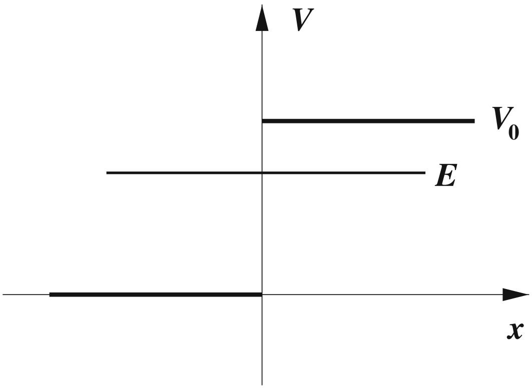

Fig. 11.1 The example of the step-like potential energy analyzed in Sect. 11.2. Only the case $0 \le E \le V_0$ is shown

11.2.1 *Case A:* $0 < E < V_0$

The Schrödinger equation is split over the two partial domains to yield

$$\begin{cases} x < 0: & -w'' = k^2 w, & k = \sqrt{2mE}/\hbar \\ x > 0: & w'' = \alpha^2 w, & \alpha = \sqrt{2m(V_0 - E)}/\hbar \end{cases} \tag{11.1}$$

where the derivatives are indicated with primes. The solutions on the left and right of the origin are respectively given by

$$w = \begin{cases} w_- = a_1 \exp(\mathrm{i}kx) + a_2 \exp(-\,\mathrm{i}kx), & x < 0 \\ w_+ = a_3 \exp(-\,\alpha x) + a_4 \exp(\alpha x), & x > 0 \end{cases} \tag{11.2}$$

where it must be set $a_4 = 0$ to prevent w_+ from diverging. Using the continuity of w and w' in the origin yields

$$\begin{cases} w_+(0) = w_-(0), & a_1 + a_2 = a_3 \\ w'_+(0) = w'_-(0), & \mathrm{i}k(a_2 - a_1) = \alpha a_3 \end{cases} \tag{11.3}$$

Eliminating a_3 provides the relation $\alpha(a_1 + a_2) = \mathrm{i}k(a_2 - a_1)$ whence

$$\frac{a_2}{a_1} = \frac{\mathrm{i}k + \alpha}{\mathrm{i}k - \alpha} = \frac{k - \mathrm{i}\alpha}{k + \mathrm{i}\alpha}, \qquad \frac{a_3}{a_1} = 1 + \frac{a_2}{a_1} = \frac{2k}{k + \mathrm{i}\alpha}, \tag{11.4}$$

that determine a_2, a_3 apart from the arbitrary constant a_1. This should be expected as w is not normalizable. From $|a_2/a_1| = |k - \mathrm{i}\alpha|/|k + \mathrm{i}\alpha| = 1$ one finds $a_2/a_1 = \exp(-\,\mathrm{i}\varphi)$, with $\varphi = 2\arctan(\alpha/k)$. The solution of the time-independent Schrödinger equation is then recast as

$$w = \begin{cases} w_- = 2a_1 \exp(-\,\mathrm{i}\varphi/2)\cos(kx + \varphi/2), & x < 0 \\ w_+ = [2k/(k + \mathrm{i}\alpha)]a_1 \exp(-\,\alpha x), & x > 0 \end{cases} \tag{11.5}$$

The eigenvalues E are continuous in the range $0 \le E < V_0$. The monochromatic wave function corresponding to w_k is $\psi_k(x,t) = w(x)\exp(-\,\mathrm{i}E_k t/\hbar)$, with $E_k = \hbar^2 k^2/(2m)$.

The quantity $R = |a_2/a_1|^2$ is called *reflection coefficient* of the monochromatic wave. As shown in Sect. 11.4 from a more general point of view, R is the probability that the wave is reflected by the step. In the case investigated here, where a particle with $0 < E < V_0$ is launched towards a step, it is $a_2/a_1 = \exp(-\,\mathrm{i}\varphi)$ whence $R = 1$.

The solution (11.3) or (11.5) shows that w becomes vanishingly small on the right of the origin as $x \to +\infty$. When a wave packet is built up using a superposition of monochromatic solutions, chosen in such a way that each energy E_k is smaller than V_0, its behavior is similar; as a consequence, the probability of finding the particle on the right of the origin becomes smaller and smaller as the distance from the origin increases. In conclusion, if a particle described by such a packet is launched from $x < 0$ towards the step, the only possible outcome is the same as in a calculation based on Classical Mechanics, namely, a reflection. A difference between the classical and quantum treatment exists though: in the former the reflection occurs at $x = 0$, whereas in the latter the reflection abscissa is not defined. This is better understood by considering a wave packet of standard deviation Δx approaching the origin from $x < 0$. Considering the approximate form of the packet described in Sect. 9.6, the incident envelope has the form $A_i = A(x - ut)$, and the localization of the incident particle is described by $|\psi_i|^2 = |A_i|^2$. Due to its finite width, the packet crosses the origin during a time $\Delta t \sim \Delta x/u$ starting, e.g., at $t = 0$. At a later instant $\Delta t + t_0$, where $t_0 \ge 0$ is the time that the wave packet takes to move away from the step to the extent that the interaction with it is practically completed, only the reflected packet exists, described by $|\psi_r|^2 = |A_r|^2$, with $A_r = A[x + u(t - t_0)]$. For $0 \le t \le \Delta t + t_0$ both incident and reflected packets exist. One could think that the reflection abscissa is given by the product ut_0; however, t_0 depends on the form of the packet, so the reflection abscissa is not well defined. Before the particle starts interacting with the step, only the incident packet exists and the normalization $\int_{-\infty}^{0} |\psi_i|^2 \mathrm{d}x = 1$ holds; similarly, after the interaction is completed, only the reflected packet exists and $\int_{-\infty}^{0} |\psi_r|^2 \mathrm{d}x = 1$. For $0 \le t \le \Delta t + t_0$ the normalization is achieved by a superposition of the incident and reflected packets.

11.2.2 Case B: $E > V_0$

Still considering the one-dimensional step of Fig. 11.1, let $E > V_0$. In this case the time-independent Schrödinger equation reads

$$\begin{cases} x < 0: \qquad -w'' = k^2 w, \qquad k = \sqrt{2m\,E}/\hbar \\ x > 0: \qquad -w'' = k_1^2 w, \qquad k_1 = \sqrt{2m(E - V_0)}/\hbar \end{cases} \tag{11.6}$$

whose solution is

$$w = \begin{cases} w_- = a_1 \exp(\mathrm{i}kx) + a_2 \exp(-\,\mathrm{i}kx), & x < 0 \\ w_+ = a_3 \exp(\mathrm{i}k_1 x) + a_4 \exp(-\,\mathrm{i}k_1 x), & x > 0 \end{cases} \tag{11.7}$$

Remembering the discussion of Sect. 9.6, function w_- in (11.7) describes a superposition of two planar and monochromatic waves, belonging to the $x < 0$ region, that propagate in the forward and backward direction, respectively; a similar meaning holds for w_+ with reference to the $x > 0$ region. Now one assumes that an extra information is available, namely, that the particle was originally launched from $x < 0$ towards the origin; it follows that one must set $a_4 = 0$, because a wave that propagates in the backward direction can not exist in the region $x > 0$. By the same token one should set $a_1 = 0$ if the particle were launched from $x > 0$ towards the origin. From the continuity of w and w' in the origin it follows

$$\begin{cases} w_+(0) = w_-(0), & a_1 + a_2 = a_3 \\ w'_+(0) = w'_-(0), & k(a_1 - a_2) = k_1 a_3 \end{cases} \tag{11.8}$$

Eliminating a_3 yields $k_1(a_1 + a_2) = k(a_1 - a_2)$ whence

$$\frac{a_2}{a_1} = \frac{k - k_1}{k + k_1}, \qquad \frac{a_3}{a_1} = 1 + \frac{a_2}{a_1} = \frac{2k}{k + k_1}, \tag{11.9}$$

that determine a_2, a_3 apart from the arbitrary constant a_1. The eigenvalues are continuous in the range $E > V_0$. The monochromatic, time-dependent wavefunction reads

$$\psi = \begin{cases} \psi_- = w_- \exp(-\,\mathrm{i}E_- t/\hbar), & x < 0 \\ \psi_+ = w_+ \exp(-\,\mathrm{i}E_+ t/\hbar), & x > 0 \end{cases} \tag{11.10}$$

where $E_- = E(k) = \hbar^2 k^2/(2m)$ and $E_+ = E(k_1) = \hbar^2 k_1^2/(2m) + V_0$. Note that $k > k_1 > 0$, namely, the modulus of the particle's momentum in the $x > 0$ region is smaller than in the $x < 0$ region; this is similar to what happens in the classical treatment. On the other hand, from $k > k_1$ it follows $a_2 \neq 0$, showing that a monochromatic plane wave propagating in the backward direction exists in the $x < 0$ region. In other term, a finite probability of reflexion is present, which whould be impossible in the classical treatment. As before, the reflection coefficient of the monochromatic wave is defined as $R = |a_2/a_1|^2 < 1$. In turn, the *transmission coefficient* is defined as $T = 1 - R$ whence, from (11.9),

$$R = \left|\frac{a_2}{a_1}\right|^2 = \frac{(k - k_1)^2}{(k + k_1)^2}, \qquad T = \frac{4kk_1}{(k + k_1)^2} = \frac{k_1}{k}\left|\frac{a_3}{a_1}\right|. \tag{11.11}$$

Like in the $0 < E < V_0$ case one may build up a wave packet of standard deviation Δx. Still considering a packet approaching the origin from $x < 0$, the envelope has the form $A_i = A(x - ut)$. Before the particle starts interacting with the step, its localization is given by $|\psi_i|^2 = |A_i|^2$. The packet crosses the origin in a time $\Delta t \sim \Delta x/u$ and, using the symbols k_0, k_{10} to indicate the center of the packet in the momentum space for $x < 0$ and $x > 0$, respectively, from the first of (11.11) the reflected packet is described by

$$|\psi_r|^2 = \frac{(k_0 - k_{10})^2}{(k_0 + k_{10})^2}|A(x + ut)|^2. \tag{11.12}$$

It has the same group velocity, hence the same width, as $|\psi_i|^2$. The transmitted packet has the form

$$|\psi_t|^2 = \frac{(2k_0)^2}{(k_0 + k_{10})^2}|A(k_0 x/k_{10} - ut)|^2, \tag{11.13}$$

and its group velocity is $u_1 = \mathrm{d}x/\mathrm{d}t = k_{10}u/k_0 < u$. As all packets cross the origin in the same time interval Δt it follows $\Delta x/u = \Delta x_1/u_1$ whence $\Delta x_1 = (k_{10}/k_0)\Delta x < \Delta x$. This result shows that the transmitted packet is slower and narrower than the incident packet (if the incident packet were launched from $x > 0$ towards the origin, the transmitted packet would be faster and wider). From $\int_{-\infty}^{0} |\psi_i|^2 \mathrm{d}x = 1$ it follows

$$P_r = \int_{-\infty}^{0} |\psi_r|^2 \mathrm{d}x = \frac{(k_0 - k_{10})^2}{(k_0 + k_{10})^2}, \tag{11.14}$$

$$P_t = \frac{k_{10}}{k_0}\int_{0}^{\infty} |\psi_t|^2 \mathrm{d}\frac{k_0 x}{k_{10}} = \frac{k_{10}}{k_0}\frac{(2k_0)^2}{(k_0 + k_{10})^2} = \frac{4k_0\,k_{10}}{(k_0 + k_{10})^2}. \tag{11.15}$$

The two numbers P_r, P_t fulfill the relations $0 < P_r, P_t < 1$, $P_r + P_t = 1$, and are the reflection and transmission probabilities of the wave packet. The treatment outlined above for the case $E > V_0$ still holds when $V_0 < 0$, $E > 0$. In particular, if $V_0 < 0$ and $|V_0| \gg E$, like in Fig. 11.2, from (11.16) it turns out $P_r \simeq 1$. This result is quite different from that obtained from a calculation based on Classical Mechanics; in fact, its features are similar to those of the propagation of light across the interface between two media of different refraction index [9, Sects. 1.5,1.6]. The oddity of the result lies, instead, in the fact that term $\sqrt{2\,m}/\hbar$ cancels out in the expressions of P_r and P_t, so that one finds

$$P_r = \frac{(\sqrt{E_0} - \sqrt{E_0 - V_0})^2}{(\sqrt{E_0} + \sqrt{E_0 - V_0})^2}, \qquad P_t = \frac{\sqrt{E_0(E_0 - V_0)}}{(\sqrt{E_0} + \sqrt{E_0 - V_0})^2}, \tag{11.16}$$

with E_0 the total energy corresponding to k_0 and k_{10}. Thus, the classical result $P_r = 0$, $P_t = 1$ cannot be recovered by making, e.g., m to increase: the discontinuity in the potential energy makes it impossible to apply the Ehrenfest approximation (10.33) no matter what the value of the mass is. The same happens for the monochromatic wave: in fact, using (11.6) and replacing E_0 with E in (11.16) makes the latter equal to (11.11). To recover the classical result it is necessary to consider a potential energy whose asymptotic values 0 and V_0 are connected by a smooth function, and solve the corresponding Schrödinger equation. The classical case is then recovered by letting m increase (Prob. 11.1).

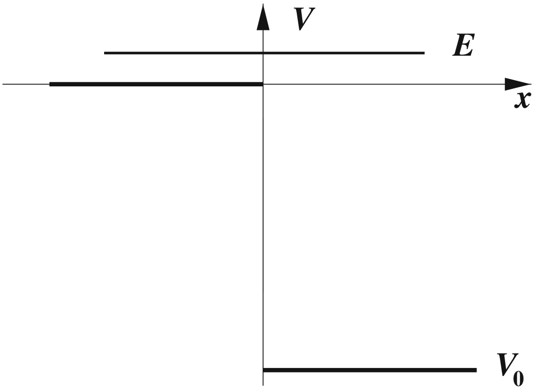

Fig. 11.2 Another example of the step-like potential energy analyzed in Sect. 11.2, with $V_0 < 0$ and $|V_0| \gg E$

11.3 Energy Barrier

Consider a one-dimensional energy barrier as shown in Fig. 11.3, with $V = V_0 > 0$ for $0 < x < s$ and $V = 0$ elsewhere. From the general properties of the time-independent Schrödinger equation (Sect. 8.2.3) it follows $E \geq 0$. To proceed, it is convenient to consider the two cases $0 < E < V_0$ and $E > V_0$ separately.

11.3.1 *Case A:* $0 < E < V_0$

The Schrödinger equation is split over the three domains to yield

$$\begin{cases} x < 0: & -w'' = k^2 w, & k = \sqrt{2m\,E}/\hbar \\ 0 < x < s: & w'' = \alpha^2 w, & \alpha = \sqrt{2\,m(V_0 - E)}/\hbar \\ s < x: & -w'' = k^2 w, & k = \sqrt{2\,m\,E}/\hbar \end{cases} \tag{11.17}$$

where the derivatives are indicated with primes. The solutions of (11.17) are, respectively,

$$w = \begin{cases} w_- = a_1 \exp(\mathrm{i}kx) + a_2 \exp(-\,\mathrm{i}kx), & x < 0 \\ w_B = a_3 \exp(\alpha x) + a_4 \exp(-\,\alpha x), & 0 < x < s \\ w_+ = a_5 \exp(\mathrm{i}kx) + a_6 \exp(-\,\mathrm{i}kx), & s < x \end{cases} \tag{11.18}$$

Using the continuity of w and w' in the origin,

$$\begin{cases} w_-(0) = w_B(0), & a_1 + a_2 = a_3 + a_4 \\ w'_-(0) = w'_B(0), & \mathrm{i}k(a_1 - a_2) = \alpha(a_3 - a_4) \end{cases} \tag{11.19}$$

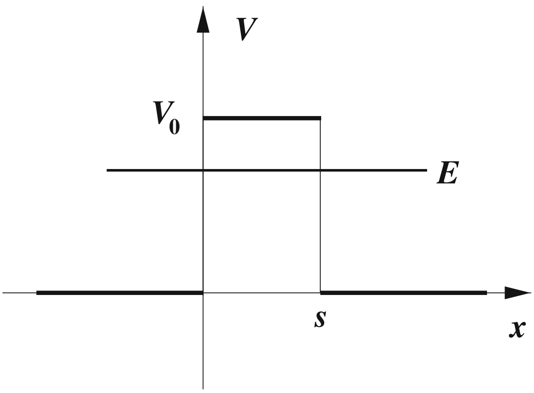

Fig. 11.3 The example of the one-dimensional energy barrier analyzed in Sect. 11.3. Only the case $0 \le E \le V_0$ is shown

Solving for a_1, a_2 and letting $\vartheta = 1 + \mathrm{i}\,\alpha/k$ yields $2\,a_1 = \vartheta\,a_4 + \vartheta^*\,a_3$, $2\,a_2 = \vartheta\,a_3 + \vartheta^*\,a_4$. Using the same reasoning as in Sect. 11.2.2, one now assumes that an extra information is available, namely, that the particle was originally launched from $x < 0$ towards the barrier; it follows that one must set $a_6 = 0$ in (11.18), because a wave that propagates in the backward direction can not exist in the region $x > s$. By the same token one should set $a_1 = 0$ if the particle were launched from $x > s$ towards the barrier. Taking the first case ($a_6 = 0$) and using the continuity of w and w' at $x = s$ provides

$$\begin{cases} w_B(s) = w_+(s), & a_3 \exp(\alpha s) + a_4 \exp(-\,\alpha s) = a_5 \exp(\mathrm{i}ks) \\ w'_B(s) = w'_+(s), & \alpha[a_3 \exp(\alpha s) - a_4 \exp(-\,\alpha s)] = \mathrm{i}ka_5 \exp(\mathrm{i}ks) \end{cases} \tag{11.20}$$

whence $2a_3 = a_5\sigma\;\exp(\mathrm{i}ks - \alpha s)$, $2a_4 = a_5\sigma^* \exp(\mathrm{i}ks + \alpha s)$, with $\sigma = 1 + \mathrm{i}k/\alpha$. In summary, a_1, a_2 are linear combinations of a_3, a_4; the latter, in turn, are proportional to a_5. It follows that, if it were $a_5 = 0$, then it would also be $a_3 = a_4 = 0$ and $a_1 = a_2 = 0$. However, this is impossible because w_- can not vanish identically; as a consequence it is necessarily $a_5 \neq 0$. This shows that $w_+ = a_5 \exp(\mathrm{i}kx)$ differs from zero, namely, that a wave propagating in the forward direction exists for $x > s$.

As the relations involving the coefficients a_i are homogeneous, they determine a_2, a_3, a_4, a_5 apart from the arbitrary constant a_1. This should be expected as w is not normalizable. As shown below, the determination of the ratios between the coefficient does not impose any constraint on the total energy; as a consequence, the eigenvalues $0 \le E < V_0$ are continuous. The ratio a_5/a_1 is found from

$$4\frac{a_1}{a_5} = 2\,\frac{a_3}{a_5}\,\vartheta^* + 2\,\frac{a_4}{a_5}\,\vartheta = \sigma\;\exp(\mathrm{i}ks - \alpha s)\vartheta^* + \sigma^* \exp(\mathrm{i}ks + \alpha s)\vartheta. \tag{11.21}$$

Letting $\mu = \vartheta\,\sigma^* = 2 + \mathrm{i}(\alpha/k - k/\alpha)$ one finds $4a_1/a_5 \exp(-\,\mathrm{i}ks) = \mu \exp(\alpha s) + \mu^* \exp(-\,\alpha s)$, whence $a_1/a_5 \exp(-\,\mathrm{i}ks) = \cosh(\alpha s) + \mathrm{i}(\alpha/k - k/\alpha)\sinh(\alpha s)/2$. Using the identity $\cosh^2\zeta - \sinh^2\zeta = 1$ finally yields for the transmission coefficient of the monochromatic wave

$$\frac{1}{T} = \left|\frac{a_1}{a_5}\right|^2 = 1 + \frac{1}{4}\left(\frac{\alpha}{k} + \frac{k}{\alpha}\right)^2 \sinh^2(\alpha s). \tag{11.22}$$

A similar calculation provides the ratio a_2/a_1; it is found

$$R = \left|\frac{a_2}{a_1}\right|^2 = \frac{(\alpha/k + k/\alpha)^2 \sinh^2(\alpha s)/4}{1 + (\alpha/k + k/\alpha)^2 \sinh^2(\alpha s)/4} = 1 - \left|\frac{a_5}{a_1}\right|^2 = 1 - T. \tag{11.23}$$

In the classical treatment, if a particle with $0 < E < V_0$ is launched from the left towards the barrier, it is reflected at $x = 0$; similarly, it is reflected at $x = s$ if it is launched from the right. In the quantum treatment it is $T > 0$: in contrast to the classical case, the particle can cross the barrier. For a given width s of the barrier and total energy E of the particle, the transmission coefficient T decreases when V_0 increases; for E and V_0 fixed, T becomes proportional to $\exp(-2\alpha s)$ when s increases to the extent that $\alpha s \gg 1$. Finally, $T \to 1$ as $s \to 0$; this was expected because the potential energy becomes equal to zero everywhere.[1]

The interaction of the particle with the barrier is better understood by considering a wave packet approaching the origin from $x < 0$. The incident envelope has the form $A_i = A(x - ut)$. Before reaching the origin the particle's localization is described by $|\psi_i|^2 = |A_i|^2$. After the interaction with the barrier is completed, both the reflected and transmitted packet exist, that move in opposite directions with the same velocity. Letting $P_r = \int_{-\infty}^{0} |\psi_r|^2 \mathrm{d}x$, $P_t = \int_s^{\infty} |\psi_t|^2 \mathrm{d}x$, and observing that $\int_{-\infty}^{0} |\psi_i|^2 \mathrm{d}x = 1$, it follows that the two numbers P_r, P_t fulfill the relations $0 < P_r, P_t < 1$, $P_r + P_t = 1$, and are the reflection and transmission probabilities of the wave packet. In summary, the solution of the Schrödinger equation for the energy barrier shows that a particle with $0 < E < V_0$ has a finite probability of crossing the barrier, which would be impossible in the classical treatment. The same result holds when the form of the barrier is more complicated than the rectangular one (Sect. 11.4). The phenomenon is also called *tunnel effect*.

11.3.2 Case B: $0 < V_0 < E$

Still considering the one-dimensional barrier of Fig. 11.3, let $0 < V_0 < E$. The Schrödinger equation over the three domains reads

[1] If the potential energy were different on the two sides of the barrier, namely, $V = V_0 > 0$ for $0 < x < s$, $V = V_L$ for $x < 0$, and $V = V_R \neq V_L$ for $x > s$, with $V_0 > V_L, V_R$, the limit $s \to 0$ would yield the case discussed in Sect. 11.2 (compare also with Sects. 11.4 and 17.8.4).

$$\begin{cases} x < 0: & -w'' = k^2 w, & k = \sqrt{2m\,E}/\hbar \\ 0 < x < s: & -w'' = k_1^2\, w, & k_1 = \sqrt{2\,m\,(E - V_0)}/\hbar \\ s < x: & -w'' = k^2\, w, & k = \sqrt{2\,m\,E}/\hbar \end{cases} \tag{11.24}$$

where the derivatives are indicated with primes. The solutions of (11.24) are, respectively,

$$w = \begin{cases} w_- = a_1 \exp(\mathrm{i}kx) + a_2 \exp(-\,\mathrm{i}kx), & x < 0 \\ w_B = a_3 \exp(\mathrm{i}k_1 x) + a_4 \exp(-\,\mathrm{i}k_1 x), & 0 < x < s \\ w_+ = a_5 \exp(\mathrm{i}kx) + a_6 \exp(-\,\mathrm{i}kx), & s < x \end{cases} \tag{11.25}$$

As in Sect. 11.3.1 one assumes that the particle was originally launched from $x < 0$, so that $a_6 = 0$. The calculation follows the same line as in Sect. 11.3.1, and yields that w_- and w_+ are the same as in (11.18), whereas w_B is found by replacing α with $\mathrm{i}k_1$ there. The determination of the ratios between the coefficient a_i does not impose any constraint on the total energy; as a consequence, the eigenvalues $E > V_0$ are continuous. Using $\cosh(\mathrm{i}\zeta) = \cos(\zeta)$, $\sinh(\mathrm{i}\zeta) = \mathrm{i}\sin(\zeta)$ then yields

$$\frac{1}{T} = \left|\frac{a_1}{a_5}\right|^2 = 1 + \frac{1}{4}\left(\frac{k}{k_1} - \frac{k_1}{k}\right)^2 \sin^2(k_1 s) \tag{11.26}$$

where, from (11.24), $k_1/k = \sqrt{1 - V_0/E}$. Similarly,

$$R = \left|\frac{a_2}{a_1}\right|^2 = \frac{(k/k_1 - k_1/k)^2 \sin^2(k_1 s)/4}{1 + (k/k_1 - k/k_1)^2 \sin^2(k_1 s)/4} = 1 - \left|\frac{a_5}{a_1}\right|^2. \tag{11.27}$$

In the classical treatment, if a particle with $0 < V_0 < E$ is launched towards the barrier, it is always transmitted. In the quantum treatment it may be $R > 0$: in contrast to the classical case, the particle can be reflected.[2] The barrier is transparent ($R = 0$) for $k_1 s = i\pi$, with i any integer. Letting $\lambda_1 = 2\pi/k_1$ yields $s = i\lambda_1/2$, which is equivalent to the optical-resonance condition in a sequence of media of refractive indices n_1, n_2, n_1 [9, Sect. 1.6].

[2] The reflection at the barrier for $k_1 s \neq i\pi$ explains why the experimental value of the Richardson constant A is lower than the theoretical one. Such a constant appears in the expression $J_s = AT^2 \exp[-E_W/(k_B T)]$ of the vacuum-tube characteristics [21]. This is one of the cases where the tunnel effect is evidenced in macroscopic-scale experiments. Still considering the vacuum tubes, another experimental evidence of the tunnel effect is the lack of saturation of the forward current-voltage characteristic at increasing bias.

11.4 Energy Barrier of a General Form

The interaction of a particle with an energy barrier has been discussed in Sect. 11.3 with reference to the simple case of Fig. 11.3. Here it is extended to the case of a barrier of a general form—still considering the one-dimensional, time-independent Schrödinger equation for a particle of mass m, to the purpose of calculating the transmission coefficient T. The equation reads

$$\frac{\mathrm{d}^2 w}{\mathrm{d}x^2} + q w = 0, \qquad q(x) = \frac{2m}{\hbar^2}\,(E - V)\,, \tag{11.28}$$

where the potential energy $V(x)$ is defined as follows:

$$V = V_L = \text{const.}, \quad x < 0; \qquad V = V_R = \text{const.}, \quad 0 < s < x. \tag{11.29}$$

In the interval $0 \le x \le s$ the potential energy is left unspecified, with the only provision that its form is such that (11.28) is solvable. It will also be assumed that $E > V_L, V_R$; as a consequence, the total energy is not quantized and all values of E larger than V_L and V_R are allowed. For a given E the time-dependent wave function takes the form $\psi(x,t) = w(x)\exp(-\,\mathrm{i}Et/\hbar)$, where

$$w(x) = a_1 \exp(\mathrm{i}k_L x) + a_2 \exp(-\,\mathrm{i}k_L x), \qquad x < 0, \tag{11.30}$$

$$w(x) = a_5 \exp(\mathrm{i}k_R x) + a_6 \exp(-\,\mathrm{i}k_R x), \qquad s < x. \tag{11.31}$$

The real parameters $k_L, k_R > 0$ are given by $k_L = \sqrt{2\,m\,(E - V_L)}/\hbar$ and, respectively, $k_R = \sqrt{2\,m\,(E - V_R)}/\hbar$. Like in the examples of Sect. 11.3 it is assumed that the particle is launched from $-\infty$, so that the plane wave corresponding to the term multiplied by a_6 in (11.31) does not exist. As a consequence one lets $a_6 = 0$, whereas a_1, a_2, a_5 are left undetermined. In the interval $0 \le x \le s$ the general solution of (11.28) is

$$w(x) = a_3\, u(x) + a_4\, v(x), \qquad 0 \le x \le s, \tag{11.32}$$

where u, v are two linearly-independent solutions. The continuity equation for the wave function, (9.13), becomes in this case $\mathrm{d}J_\psi/\mathrm{d}x = 0$, namely, $J_\psi = \text{const.}$ In turn, the density of the probability flux reads

$$J_\psi = \frac{\mathrm{i}\hbar}{2m}\left(w\frac{\mathrm{d}w^*}{\mathrm{d}x} - w^*\frac{\mathrm{d}w}{\mathrm{d}x}\right). \tag{11.33}$$

Applying (11.33) to (11.30) and (11.31) yields, respectively,

$$J_\psi = \frac{\hbar k_L}{m}\left(|a_1|^2 - |a_2|^2\right), \quad x < 0; \qquad J_\psi = \frac{\hbar k_R}{m}|a_5|^2, \quad s < x. \tag{11.34}$$

As J_ψ is constant, one may equate the two expressions in (11.34) to obtain

$$\left|\frac{a_2}{a_1}\right|^2 + \frac{k_R}{k_L}\left|\frac{a_5}{a_1}\right|^2 = 1. \tag{11.35}$$

The division by $|a_1|^2$ leading to (11.35) is allowed because, by hypotesis, the particle is launched from $-\infty$, so that $a_1 \neq 0$. From (11.35) one defines the reflection and transmission coefficients

$$R = \left|\frac{a_2}{a_1}\right|^2, \qquad T = \frac{k_R}{k_L}\left|\frac{a_5}{a_1}\right|^2. \tag{11.36}$$

Given E, V_L, V_R, and a_1, the transmission and reflection coefficients depend on the form of the potential energy in the interval $0 \leq x \leq s$. By way of example, if $V_L = 0$ and the potential energy in the interval $0 \leq x \leq s$ is equal to some constant $V_B \geq 0$, then R is expected to vary from 0 to 1 as V_B varies from 0 to $+\infty$. On the other hand, R and T can not vary independently from each other because of the relation $R + T = 1$. As a consequence, it suffices to consider only one coefficient, say, T. From the discussion above it follows that the coefficient T depends on the shape of the potential energy that exists within the interval $0 \leq x \leq s$, namely, it is a functional of V: $0 \leq T = T[V] \leq 1$. One may also note that the relation $R + T = 1$ derives only from the constancy of J_ψ due to the one-dimensional, steady-state condition. In other terms, the relation $R + T = 1$ does not depend on the form of the potential energy within the interval $0 \leq x \leq s$. It must then reflect some invariance property intrinsic to the solution of the problem. In fact, the invariance is that of the density of the probability flux J_ψ, which is intrinsic to the form of the Schrödinger equation and leads to the relation (11.35).

For the sake of generality one provisionally considers a slightly more general equation than (11.28), built by the linear operator

$$\mathcal{L} = \frac{\mathrm{d}^2}{\mathrm{d}x^2} + p(x)\frac{\mathrm{d}}{\mathrm{d}x} + q(x), \tag{11.37}$$

where the functions p and q are real. If u is a solution of the differential equation $\mathcal{L}w = 0$ in the interval $0 \leq x \leq s$, let $P(x)$ be any function such that $p = \mathrm{d}P/\mathrm{d}x$, and define

$$v(x) = u(x)\int_a^x \frac{\exp[-P(\xi)]}{u^2(\xi)}\mathrm{d}\xi, \tag{11.38}$$

where a, x belong to the same interval. It is found by inspection that $\mathcal{L}v = 0$ in the interval $0 \leq x \leq s$, namely, v is also a solution. Moreover, the Wronskian of u and v (Sect. A.12) reads

$$W(x) = uv' - u'v = \exp(-P). \tag{11.39}$$

As the Wronskian never vanishes, u and v are linearly independent. This shows that, for any solution u of the differential equation $\mathcal{L}w = 0$ in a given interval, (11.38) provides another solution which is linearly independent from u. As the differential equation is linear and of the second order, the general solution is then given by a linear combination of u and v.

Being the equation $\mathcal{L}w = 0$ homogeneous, the solution u may be replaced by λu, with $\lambda \neq 0$ a constant. In this case v must be replaced by v/λ due to (11.38).

It follows that the Wronskian (11.39) is invariant under scaling of the solutions. Another consequence of the homogeneity of $\mathcal{L}w = 0$ is that the dimensions of w may be chosen arbitrarily. The same holds for the dimensions of u. Once the latter have been chosen, the dimensions of v follow from (11.38); in fact, the product uv has the dimensions of a length. From (11.32) it then follows that the products $a_3 u$ and $a_4 v$ have the same dimensions.

The linear independency allows one to choose for u and v the two fundamental solutions, namely, those having the properties [51, Sect. 5.2]

$$u(0) = 1, \qquad u'(0) = 0, \qquad v(0) = 0, \qquad v'(0) = 1, \tag{11.40}$$

so that the Wronskian W equals 1 everywhere. Then, letting $a_6 = 0$ in (11.31) and prescribing the continuity of the solution and its derivative at $x = 0$ and $x = s$ yields, from (11.32),

$$a_3 = a_1 + a_2, \qquad a_4 = \mathrm{i}k_L(a_1 - a_2), \tag{11.41}$$

$$a_5 \exp(jk_R s) = a_3 u_s + a_4 v_s, \qquad \mathrm{i}k_R a_5 \exp(\mathrm{i}k_R s) = a_3 u'_s + a_4 v'_s, \tag{11.42}$$

where suffix s indicates that the functions are calculated at $x = s$. Eliminating $a_5 \exp(\mathrm{i}\, k_R\, s)$ yields $(\mathrm{i}\, k_R\, u_s - u'_s)\, a_3 = (v'_s - \mathrm{i}\, k_R\, v_s)\, a_4$ whence, from (11.41),

$$\frac{a_2}{a_1} = \frac{k_L k_R v_s + u'_s + j\,(k_L\, v'_s - k_R\, u_s)}{k_L k_R v_s - u'_s + j\,(k_L\, v'_s + k_R\, u_s)} = \frac{A + jB}{C + jD}. \tag{11.43}$$

In conclusion, $T = 1 - |a_2/a_1|^2 = (C^2 - A^2 + D^2 - B^2)/(C^2 + D^2)$. Using $W = 1$ transforms the numerator into $C^2 - A^2 + D^2 - B^2 = 4k_L k_R (u_s v'_s - v_s u'_s) = 4k_L k_R$. In turn, the denominator reads $C^2 + D^2 = 2k_L k_R + (k_R u_s)^2 + (u'_s)^2 + (k_L v'_s)^2 + (k_L k_R v_s)^2$, whence

$$T = \frac{4k_L k_R}{2k_L k_R + (k_R u_s)^2 + (u'_s)^2 + (k_L v'_s)^2 + (k_L k_R v_s)^2}. \tag{11.44}$$

The expression of the transmission coefficient may be recast as $T = 1/(1 + F)$, with

$$F = \frac{1}{4k_L k_R}\left[\left(u'_s\right)^2 + (k_R u_s)^2\right] + \frac{k_L}{4k_R}\left[\left(v'_s\right)^2 + (k_R v_s)^2\right] - \frac{1}{2}. \tag{11.45}$$

It is easily shown that $F > 0$; in fact, this condition is equivalent to $(k_R u_s - k_L v'_s)^2 + (u'_s + k_L k_R v_s)^2 > 0$. In conclusion, (11.44) is the expression of the transmission coefficient across a barrier of any form, with no approximation [88]. To calculate T it is necessary to determine the four quantities u_s, u'_s, v_s, and v'_s. Actually only three of them suffice thanks to the condition $u_s v'_s - u'_s v_s = 1$.

Repeating the calculation of this section after letting $a_1 = 0$, $a_6 \neq 0$ provides the known result that, for a given barrier, the transmission probability for a particle of energy E is the same whether the particle is launched from the left or from the right. The property holds also in the relativistic case [79].

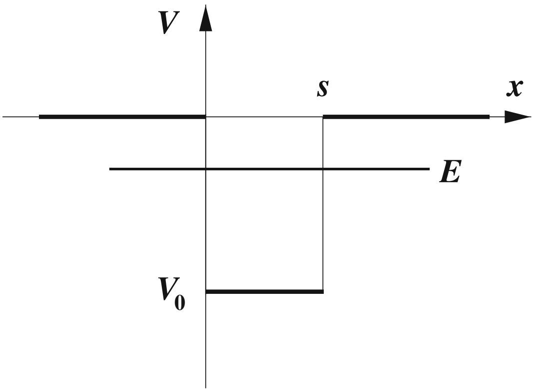

Fig. 11.4 The example of the one-dimensional energy well analyzed in Sect. 11.5. Only the case $V_0 < E < 0$ is shown

11.5 Energy Well

Taking a one-dimensional case, let $V = V_0 < 0$ for $0 < x < s$ and $V = 0$ elsewhere. From the general properties of the time-independent Schrödinger equation it follows $E > V_0$. The case $E > 0$ is treated in the same way as that of Sect. 11.3.2 and leads to similar results. The case $V_0 < E < 0$, shown in Fig. 11.4, is instead different from those investigated above: the total energy is quantized and the wave function is square integrable. The Schrödinger equation over the three domains reads

$$\begin{cases} x < 0: & w'' = \alpha^2 w, & \alpha = \sqrt{-2\,m\,E}/\hbar \\ 0 < x < s: & -w'' = k^2\,w, & k = \sqrt{2\,m\,(E - V_0)}/\hbar \\ s < x: & w'' = \alpha^2\,w, & \alpha = \sqrt{-2\,m\,E}/\hbar \end{cases} \tag{11.46}$$

where the derivatives are indicated with primes. The solutions of (11.46) are, respectively,

$$w = \begin{cases} w_- = a_1 \exp(\alpha x) + a_5 \exp(-\,\alpha x), & x < 0 \\ w_W = a_2 \exp(\mathrm{i}kx) + a_3 \exp(-\,\mathrm{i}kx), & 0 < x < s \\ w_+ = a_4 \exp(-\,\alpha x) + a_6 \exp(\alpha x), & s < x \end{cases} \tag{11.47}$$

where it must be set $a_5 = a_6 = 0$ to prevent w_- and w_+ from diverging. Using the continuity of w and w' in the origin,

$$\begin{cases} w_-(0) = w_W(0), & a_1 = a_2 + a_3 \\ w'_-(0) = w'_W(0), & \alpha a_1 = \mathrm{i}k(a_2 - a_3) \end{cases} \tag{11.48}$$

Solving for a_2, a_3 and letting $\vartheta = 1 + \mathrm{i}\alpha/k$ yields $2a_2 = \vartheta^* a_1$, $2a_3 = \vartheta a_1$ whence $a_2/a_3 = \vartheta^*/\vartheta$. Then, using the continuity of w and w' at $x = s$ yields

$$\begin{cases} w_W(s) = w_+(s), & a_4 \exp(-\alpha s) = a_2 \exp(\mathrm{i}ks) + a_3 \exp(-\mathrm{i}ks) \\ w'_W(s) = w'_+(s), & -\alpha a_4 \exp(-\alpha s) = \mathrm{i}k[a_2 \exp(\mathrm{i}ks) - a_3 \exp(-\mathrm{i}ks)] \end{cases}$$

Solving for a_2, a_3 yields $2a_2 = a_4 \vartheta \exp(-\alpha s - \mathrm{i}ks)$, $2a_3 = a_4 \vartheta^* \exp(-\alpha s + \mathrm{i}ks)$, whence $a_2/a_3 = (\vartheta/\vartheta^*) \exp(-2\mathrm{i}ks)$. In summary, a_2, a_3 are proportional to a_1 and to a_4. It follows that, if it were $a_1 = 0$ or $a_4 = 0$, then it would also be $a_2 = a_3 = 0$. However, this is impossible because w can not vanish identically; as a consequence it is necessarily $a_1 \neq 0$, $a_4 \neq 0$. This shows that, in contrast to the classical case, the particle penetrates the boundaries of the well. The relations found so far determine two different expressions for a_2/a_3. For them to be compatible, the equality $\vartheta^2 \exp(-\mathrm{i}ks) = (\vartheta^*)^2 \exp(\mathrm{i}ks)$ must hold, which represents the condition of a vanishing determinant of the 4×4, homogeneous algebraic system whose unknowns are a_1, a_2, a_3, and a_4. Using $\vartheta = 1 + \mathrm{i}\alpha/k$, the equality is recast as

$$\left(1 - \frac{\alpha^2}{k^2}\right) \sin(ks) = 2\frac{\alpha}{k} \cos(ks), \qquad \frac{k^2 - \alpha^2}{2\alpha k} = \cot(ks). \tag{11.49}$$

Finally, replacing the expressions of α and k provides the transcendental equation

$$\frac{E - V_0/2}{\sqrt{-E(E - V_0)}} = \cot\left(s\frac{\sqrt{2m}}{\hbar}\sqrt{E - V_0}\right), \qquad V_0 < E < 0, \tag{11.50}$$

in the unknown E, whose roots fulfill the compatibility condition. As a consequence, such roots are the eigenvalues of E. Given m, s, and V_0, let $n \geq 1$ be an integer such that

$$(n-1)\pi < s\sqrt{-(2m/\hbar^2)V_0} \leq n\pi. \tag{11.51}$$

Such an integer always exists, and indicates the number of branches of $\cot(ks)$ that belong (partially or completely) to the interval $V_0 < E < 0$. In such an interval the left hand side of (11.50) increases monotonically from $-\infty$ to $+\infty$; as a consequence, (11.50) has n roots $V_0 < E_1, E_2, \ldots, E_n < 0$. An example with five roots is shown in Fig. 11.5; the corresponding calculation is carried out in Prob. 11.2. When an eigenvalue, say E_i, is introduced into (11.46), it provides α_i, k_i, and $\vartheta_i = 1 + \mathrm{i}\alpha_i/k_i$; in conclusion,

$$a_{i2} = \frac{1}{2}\vartheta_i^* a_{i1}, \qquad a_{i3} = \frac{1}{2}\vartheta_i a_{i1}, \qquad a_{i4} = \frac{\vartheta_i^*}{\vartheta_i} \exp(\alpha_i s + \mathrm{i}k_i s) a_{i1}. \tag{11.52}$$

The ith eigenfunction w_i can thus be expressed, from (11.50), in terms of a_{i1} alone. The latter, in turn, is found from the normalization condition $\int_{-\infty}^{+\infty} |w_i|^2 \mathrm{d}x = 1$.

The case of the box treated in Sect. 8.2.2 is obtained by letting $V_0 \to -\infty$ here; at the same time one lets $E \to -\infty$ in such a way that the difference $E - V_0$ is kept finite. In this way, w_- and w_+ in (11.47) vanish identically and yield the boundary conditions for w_W used in Sect. 8.2.2.

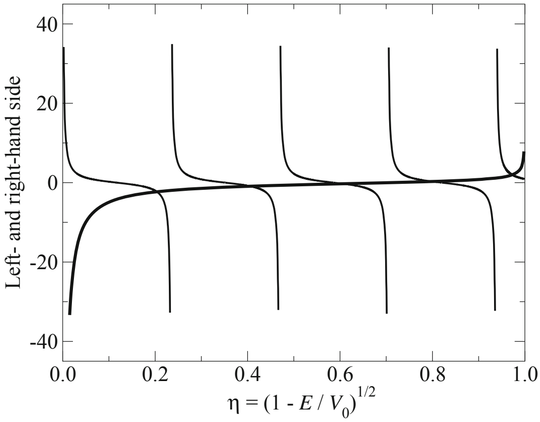

Fig. 11.5 Graphic solution of (11.50) using the auxiliary variable η. The solutions $\eta_1, \ldots, \eta_5$ are the intercepts of the left hand side (thicker line) with the branches of the right hand side. The data are given in Prob. 11.2

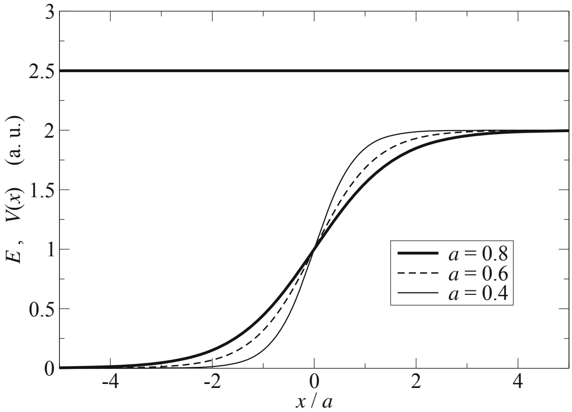

Fig. 11.6 The smooth potential energy considered in Prob. 11.1, with $V_0 = 2$ and $E = 2.5$ (arbitrary units).

Problems

11.1 Consider a smooth potential energy described by

$$V(x) = \frac{V_0}{1 + \exp(-x/a)}, \tag{11.53}$$

with $V_0 > 0$, $a > 0$ (Fig. 11.6). The limit of $V(x)$ for $a \to 0$ yields the discontinuous step of Sect. 11.2. Considering a monochromatic wave with $E > V_0$ launched from the left towards the barrier, the reflection coefficient is found to be [41, Sect. 2.2].

$$R(a) = \frac{\sinh^2 [\pi a \sqrt{2m}(\sqrt{E} - \sqrt{E - V_0})/\hbar]}{\sinh^2 [\pi a \sqrt{2m}(\sqrt{E} + \sqrt{E - V_0})/\hbar]}. \tag{11.54}$$

Discuss the limiting cases $a \to 0$ and $m \to \infty$ and compare the results with those found in Sect. 11.2.

11.2 Find the eigenvalues of the Schrödinger equation for an energy well like that of Fig. 11.5, having a width $s = 15$ Å $= 1.5 \times 10^{-9}$ m and a depth[3] $-V_0 = 3$ eV $\simeq 4.81 \times 10^{-19}$ J. Use $m \simeq 9.11 \times 10^{-31}$ kg, $\hbar \simeq 1.05 \times 10^{-34}$ J s.

[3] The *electron Volt* (eV) is a unit of energy obtained by multiplying 1 J by a number equal to the modulus of the electron charge expressed in C (Table D.1).