2.4 Potential Step

As a first illustration of the use of Schrödinger's equation, let us determine the wave function \( \psi(x) \) for a particle moving in a region in which the potential energy is as illustrated in Fig. 2-3; this situation is called a potential step. That is, the potential energy is zero for \( x < 0 \) and has the constant value \( E_0 \) for \( x > 0 \). No physical potential exhibits such an abrupt or sudden change; it is more reasonable to expect the change in potential to be smooth, as shown by the dashed line. For example, free electrons in a metal experience this smooth change of potential near the metal surface. However, the nonphysical potential step is mathematically simpler and its results are applicable to actual cases, as an indication of the physical situation. It is necessary to consider separately the cases for which \( E < E_0 \) and for which \( E > E_0 \).

![Figure 2-3. Potential step. (In this and all succeeding figures the classically forbidden regions are shaded.)](image)

(a) \( E < E_0 \). In this case, classical mechanics tells us that the particle cannot be to the right of \( O \), because then the kinetic energy \( E_k = E - E_0 \) would be negative, which is impossible. Thus \( x > 0 \) is a classically forbidden region if \( E < E_0 \). This means that, in the case of free electrons in a metal, those electrons with \( E < E_0 \) cannot escape from the metal; when they reach the surface of the metal, they are turned back into it.
To obtain \( \psi(x) \) for a potential step we must write Schrödinger's equation separately for the regions \( x < 0 \) (or I) and \( x > 0 \) (or II). In region (I), in which \( E_p = 0 \), Eq. (2.3) becomes

\[
\frac{d^2 \psi_1}{dx^2} + \frac{2mE}{\hbar^2} \psi_1 = 0,
\]

which is identical to Eq. (2.4) for a free particle. Its general solution is of the type given in Eq. (2.7), or

\[
\psi_1(x) = Ae^{ikx} + Be^{-ikx}. \tag{2.10}
\]

In the way it is written it represents an incident particle \( e^{ikx} \) and a reflected particle \( e^{-ikx} \). We are assigning a different amplitude to the reflected particle to take into account any possible change of the incident beam as a result of the reflection at \( x = 0 \). In region (II), in which \( E_p(x) = E_0 \), Schrödinger's equation is

\[
\frac{d^2 \psi_2}{dx^2} + \frac{2m(E - E_0)}{\hbar^2} \psi_2 = 0. \tag{2.11}
\]

When \( E < E_0 \), we may define the positive quantity \( \alpha^2 = 2m(E - E_0)/\hbar^2 \), so that the differential equation (2.11) becomes

\[
\frac{d^2 \psi_2}{dx^2} - \alpha^2 \psi_2 = 0.
\]

The solution of this differential equation is a combination of the functions \( e^{\alpha x} \) and \( e^{-\alpha x} \), as we may verify by direct substitution. But the increasing function \( e^{\alpha x} \) is not acceptable because we know that the field amplitude is very small in region (II); experience tells us that we are not likely to find a particle in that region (recall our statement that, classically speaking, it is impossible). Therefore we must use only the decreasing exponential function \( e^{-\alpha x} \), or

\[
\psi_2(x) = Ce^{-\alpha x}.
\]

The fact that \( \psi_2(x) \) is not zero means that there is some probability of finding the particle in region (II). This constitutes one of the most interesting peculiarities that distinguish quantum from classical mechanics. That is, in quantum mechanics, the region in which a particle may move does not, in general, have sharp boundaries. However, since \( \psi(x) \) is given by a negative (or decreasing) exponential, the probability of finding the particle with \( E < E_0 \) to the right of the potential step (that is, where \( x > 0 \)), decreases very rapidly as \( x \) increases. In general, therefore, the particle cannot go very far into the classically forbidden region.

We can determine the constants \( A, B, \) and \( C \) only by applying the condition of continuity of the matter field or wave function at \( x = 0 \), which is an obvious physical requirement. That is, the wave function must change smoothly as it crosses the potential step. This requires that

\[
\psi_1 = \psi_2 \quad \text{and} \quad \frac{d\psi_1}{dx} = \frac{d\psi_2}{dx} \quad \text{for} \quad x = 0.
\]

These conditions yield \( A + B = C \) and \( ik(A - B) = -\alpha C \), which in turn give

\[
B = \frac{(ik + \alpha)A}{ik - \alpha} \quad \text{and} \quad C = \frac{2ikA}{ik - \alpha},
\]

so that

\[
\psi_1(x) = A \left( e^{ikx} + \frac{ik + \alpha}{ik - \alpha} e^{-ikx} \right), \quad \psi_2(x) = \frac{2ik}{ik - \alpha} A e^{-\alpha x}.
\]

In the form we have written \( \psi_1 \), the intensity of the incoming field is \( |A|^2 \). The intensity of the reflected field is

\[
|B|^2 = \frac{|ik + \alpha|}{|ik - \alpha|^2} = \frac{ik + \alpha}{ik - \alpha} \frac{-ik + \alpha}{-ik - \alpha} |A|^2 = |A|^2.
\]

Therefore both the incident and the reflected fields have the same intensity. We may interpret this result by saying that all particles reaching the potential step with \( E < E_0 \) bounce back, including those that penetrate slightly into region (II). This interpretation is in agreement with the physical picture of the process.

The function \( \psi_1(x) \) can also be written in the alternate form

\[
\psi_1(x) = \frac{A}{ik - \alpha} [(ik - \alpha)e^{ikx} + (ik + \alpha)e^{-ikx}]
\]

and, remembering that \( e^{\pm ikx} = \cos kx \pm i \sin kx \), we obtain after multiplication,

\[
\psi_1(x) = \frac{2ik}{ik - \alpha} A \left( \cos kx - \frac{\alpha}{k} \sin kx \right).
\]

Thus, disregarding the common complex factor \( 2ik/(ik - \alpha) \) which multiplies \( \psi_1 \) and \( \psi_2 \), we can represent both functions by the curves of Fig. 2-4. The larger the potential energy \( E_0 \), the larger the value of \( \alpha \) and the faster the function \( \psi_2 \) goes to zero for \( x > 0 \) for a given energy \( E \). In the limit as \( E_0 \) becomes very large,
so that $\alpha$ is also very large, the function $\psi_2$ is essentially identical to zero ($\psi_2 = 0$), and no particle can penetrate into the classically forbidden region at the right ($x > 0$). In other words, all particles are reflected at $x = 0$. In this case, the above expression for $\psi_1$ becomes

$$\psi_1 = 2iA \sin kx = C \sin kx,$$

as indicated in Fig. 2-5. (The student should compare this situation with that of waves on a string with a fixed end.)

![Fig. 2-5. (a) Potential wall. The particle cannot penetrate the region $x > 0$. (b) Wave function for a potential wall.](image)

(b) $E > E_0$. In this case, if we again assume that the particles come from the left, the classical description would be that all particles proceed into region (II), although they move with a smaller velocity than in region (I). At $x = 0$ the particles suffer a sudden deceleration, since their kinetic energy is smaller in (II) than in (I). The quantum-mechanical picture is different. The solution for region (I) is still given by Eq. (2.10), $\psi_1 = Ae^{ikx} + Be^{-ikx}$, if we assume that it is possible that some particles are reflected (an assumption which we shall verify later). However, for region (II) the solution is different, because now $E > E_0$ and we must define the positive quantity $k' = \sqrt{2m(E - E_0)/\hbar^2}$ so that Eq. (2.11) becomes

$$\frac{d^2\psi_2}{dx^2} + k'^2\psi_2 = 0.$$

The solution is now also similar to the solution of Eq. (2.7). One thing is certain in this case; in region (II) we have particles traveling only to the right, and thus we must write

$$\psi_2(x) = Ce^{ik'x}.$$  \hspace{1cm} (2.12)

Applying the boundary conditions at $x = 0$ to the functions given by Eqs. (2.10) and (2.12), we then have

$$A + B = C, \quad k(A - B) = k'C;$$

whose solutions are $B = (k - k')A/(k + k')$ and $C = 2kA/(k + k')$, so that

$$\psi_1(x) = A \left( e^{ikx} + \frac{k - k'}{k + k'} e^{-ikx} \right), \quad \psi_2(x) = \frac{2k}{k + k'} Ae^{ik'x}.$$

The fact that $B$ is not zero is an indication that some particles are reflected at $x = 0$, which again is a result different from that predicted by classical mechanics. This reflection is a characteristic behavior of all fields whenever, in their propagation, they encounter a region of discontinuity in the physical properties of the medium. This behavior is well known for the case of elastic and electromagnetic waves.

**EXAMPLE 2.2.** Determine the reflection and the transmission coefficients of the potential step for $E > E_0$.

**Solution:** Let us call $v = p/m = \hbar k/m$ the velocity of the particle in region (I) and $v' = \hbar k'/m$ the velocity in region (II). Recall that the intensity of the incoming particles (that is, the number of particles per unit volume in the incident beam) is given by $|A|^2$. Then the "flux" of the incoming beam or particle current density (that is, the number of particles passing through a unit area per unit time) is $|A|^2$. The "flux" of the reflected field is $|B|^2$, since the speed remains the same for the reflected field, and that of the transmitted field is $|C|^2$. Thus the reflection and transmission coefficients are

$$R = \frac{|B|^2}{|A|^2} = \frac{(k - k')^2}{k + k'^2},$$

$$T = \frac{|C|^2}{|A|^2} = \frac{k'^2}{k(k + k')} = \frac{4kk'}{(k + k')^2}.$$

Both $R$ and $T$ are smaller than 1, since the incoming beam of particles is split into reflected and transmitted beams. The student should verify that $R + T = 1$, which is required for conservation of the number of particles, since the incoming flux of particles must be equal to the sum of those reflected and those transmitted.

### 2.5 Particle in a Potential Box

Consider, as a second example, the case of a particle constrained to move in the region from $x = 0$ to $x = a$, such as a gas molecule in a box. The molecule moves freely until it hits the wall, which forces the molecule to bounce back. A similar situation exists for a free electron in a piece of metal, if we neglect the electron's interactions with the positive ions and if the height of the potential barrier is much larger than the electron's kinetic energy. The electron can move freely through the metal but cannot escape from it.