changes by only a small amount in a distance as short as a de Broglie wavelength. So it is also not necessary, in that limit, to speak of averages when discussing potentials. Thus, in the macroscopic limit we can ignore the bars representing expectation values, or averages, in the equations just displayed. We then conclude that *Newton's law of motion can be derived from the Schroedinger equation, in the classical limit of macroscopic systems. Newton's law of motion is a special case of Schroedinger's equation.*

6-3 The Step Potential (Energy Less Than Step Height)

In the next sections we shall study solutions to the time-independent Schroedinger equation for a particle whose potential energy can be represented by a function $V(x)$ which has a different constant value in each of several adjacent ranges of the x axis. These potentials change in value abruptly in going from one range to the adjacent range. Of course potentials which change abruptly (i.e., are discontinuous functions of x) do not really exist in nature. Nevertheless, these idealized potentials are used frequently in quantum mechanics to approximate real situations because, being constant in each range, they are easy to treat mathematically. The results we obtain for these potentials will allow us to illustrate a number of characteristic quantum mechanical phenomena.

An analogy, that is surely familiar to the student, is found in the procedure used in studying electromagnetism. This involves treating many idealized systems like the infinite wire, the capacitor without edges, etc. These systems are studied because they are relatively easy to handle, because they are excellent approximations to real ones, and because real systems are usually complicated to treat mathematically since they have complicated geometries. The idealized potentials we treat in this chapter are used in the same way and with the same justification.

The simplest case is the *step potential*, illustrated in Figure 6-3. If we choose the origin of the x axis to be at the step, and the arbitrary additive constant that always occurs in the definition of a potential energy so that the potential energy of the particle is zero when it is to the left of the step, $V(x)$ can be written

$$V(x) = \begin{cases} V_0 & x > 0 \\ 0 & x < 0 \end{cases} \tag{6-11}$$

where V_0 is a constant. We may think of $V(x)$ as an approximate representation of the potential energy function for a charged particle moving along the axis of a system of two electrodes, separated by a very narrow gap, which are held at different voltages. The upper half of Figure 6-4 illustrates this system, and the lower half illustrates the corresponding potential energy function. As the gap decreases, the potential function approaches the idealization illustrated in Figure 6-3. In Example 6-2 we shall see that the potential energy for an electron moving near the surface of a metal is very much like a step potential since it rapidly increases at the surface from an essentially constant interior value to a higher constant exterior value.

Assume that a particle of mass m and total energy E is in the region $x < 0$, and that it is moving toward the point $x = 0$ at which the step potential $V(x)$ abruptly changes its value. According to classical mechanics, the particle will move freely in that region until it reaches $x = 0$, where it is subjected to an impulsive force $F = -dV(x)/dx$ acting in the direction of decreasing x. The idealized potential, (6-11), yields an impulsive force of infinite magnitude acting only at the point $x = 0$. However, as it acts on the particle only for an infinitesimal time, the quantity $\int F\,dt$ (the

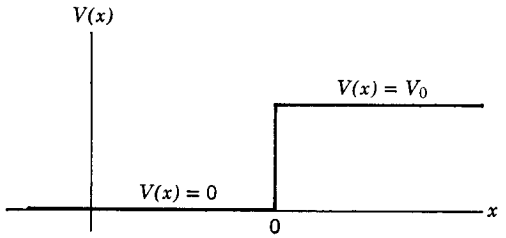


FIGURE 6-3
A step potential.

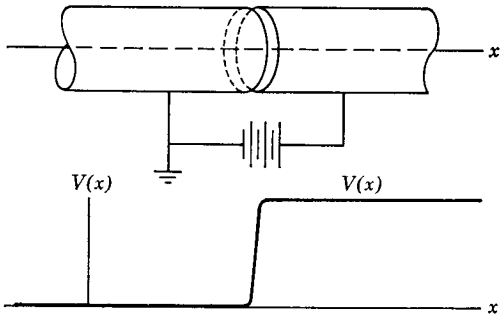


FIGURE 6-4
Illustrating a physical system with a potential energy function that can be approximated by a step potential. A charged particle moves along the axis of two cylindrical electrodes held at different voltages. Its potential energy is constant when it is inside either electrode, but it changes very rapidly when passing from one to the other.

impulse), which determines the change in its momentum, is finite. In fact, the momentum change is not affected by the idealization.

The motion of the particle subsequent to experiencing the force at $x = 0$ depends, in classical mechanics, on the relation between E and V_0. This is also true in quantum mechanics. In the present section we treat the case where $E < V_0$, i.e., where the total energy is less than the height of the potential step as illustrated in Figure 6-5. (The case where $E > V_0$ is treated in the following section.) Since the total energy E is a constant, *classical mechanics* says that the particle cannot enter the region $x > 0$. The reason is that in that region

$$E = \frac{p^2}{2m} + V(x) < V(x)$$

or

$$\frac{p^2}{2m} < 0$$

Thus the kinetic energy $p^2/2m$ would be negative in the region $x > 0$, which would lead to an imaginary value for the linear momentum p in that region. Neither is allowed, or even makes physical sense, in classical mechanics. According to classical mechanics, the impulsive force will change the momentum of the particle in such a way that it will exactly reverse its motion, traveling off in the direction of decreasing x with momentum in the direction opposite to its initial momentum. The magnitude of the momentum p will be the same before and after the reversal since the total energy $E = p^2/2m$ is constant.

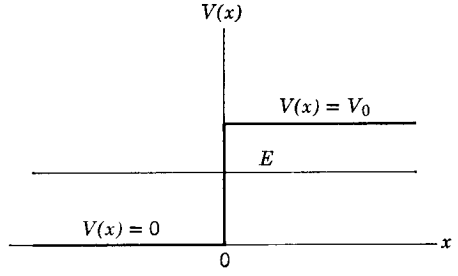


FIGURE 6-5
The relation between total and potential energies for a particle incident upon a potential step with total energy less than the height of the step.

To determine the motion of the particle according to *quantum mechanics*, we must find the wave function which is a solution, for the total energy $E < V_0$, to the Schroedinger equation for the step potential of (6-11). Since this potential is independent of time, the actual problem is to solve the time-independent Schroedinger equation. From our qualitative discussion of the previous chapter, we know that an acceptable solution should exist for *any* value of $E \geq 0$, since the potential cannot bind the particle to a limited range of the x axis.

For the step potential, the x axis breaks up into two regions. In the region where $x < 0$ (left of the step), we have $V(x) = 0$, so the eigenfunction that will tell us about the behavior of the particle is a solution to the simple time-independent Schroedinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \qquad x < 0 \quad (6\text{-}12)$$

In the region where $x > 0$ (right of the step), we have $V(x) = V_0$, and the eigenfunction is a solution to a time-independent Schroedinger equation which is almost as simple

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V_0\psi(x) = E\psi(x) \qquad x > 0 \quad (6\text{-}13)$$

The two equations are solved separately. Then an eigenfunction valid for the entire range of x is constructed by joining the two solutions together at $x = 0$ in such a way as to satisfy the requirements, of Section 5-6, that the eigenfunction and its first derivative are everywhere finite, single valued, and continuous.

Consider the differential equation valid for the region in which $V(x) = 0$, (6-12). Since this is precisely the time-independent Schroedinger equation for a free particle, we take for its *general* solution the traveling wave eigenfunction of (6-8). We write that eigenfunction as

$$\psi(x) = Ae^{ik_1x} + Be^{-ik_1x} \qquad \text{where } k_1 = \frac{\sqrt{2mE}}{\hbar} \qquad x < 0 \quad (6\text{-}14)$$

Next consider the differential equation valid for the region in which $V(x) = V_0$, (6-13). From the qualitative considerations of Section 5-7, we do not expect an oscillatory function, such as in (6-14), to be a solution since the total energy E is less than the potential energy V_0 in the region of interest. In fact, those considerations tell us that the solution will be a function which "gradually approaches the x axis." The simplest function with this property is the decreasing *real* exponential, which can be written

$$\psi(x) = e^{-k_2x} \qquad x > 0 \quad (6\text{-}15)$$

Let us find out if this is a solution and, if so, also find the required value of k_2, by substituting it into (6-13), which it is supposed to satisfy. We first evaluate

$$\frac{d^2\psi(x)}{dx^2} = (-k_2)^2e^{-k_2x} = k_2^2\psi(x)$$

Then the substitution yields

$$-\frac{\hbar^2}{2m}k_2^2\psi(x) + V_0\psi(x) = E\psi(x)$$

This satisfies the equation, and therefore verifies the solution, providing

$$k_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \qquad E < V_0 \quad (6\text{-}16)$$

The solution we have just verified is not a *general* solution to the time-independent Schroedinger equation, (6-13). The reason is that the equation contains a second derivative, so the general solution must contain two arbitrary constants. However, if we can find a solution to the equation for the same value of E, which is different in form from the one we have just found, we can make an arbitrary linear combination of these two so-called *particular* solutions. The linear combination will also be a solution and, since it will contain two arbitrary constants, it will be a general solution.

A clue to the form of another particular solution is found by noting that k_2 enters as a square in the equation preceding (6-16). Therefore, its sign is immaterial, and the increasing exponential

$$\psi(x) = e^{+k_2 x} \qquad \text{where } k_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \qquad x > 0 \quad (6\text{-}17)$$

should also be a solution to the time independent Schroedinger equation that we are dealing with. It is equally easy to verify this, by substitution into the equation. But let us instead verify that the arbitrary linear combination of the two particular solutions

$$\psi(x) = Ce^{k_2 x} + De^{-k_2 x} \qquad \text{where } k_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \qquad x > 0 \quad (6\text{-}18)$$

and where C and D are arbitrary constants, is a solution to (6-13). We calculate

$$\frac{d^2\psi(x)}{dx^2} = Ck_2^2 e^{k_2 x} + D(-k_2)^2 e^{-k_2 x} = k_2^2 \psi(x) = \frac{2m(V_0 - E)}{\hbar^2}\psi(x)$$

and substitute the result into the equation. We obtain

$$-\frac{\hbar^2}{2m}\frac{2m}{\hbar^2}(V_0 - E)\psi(x) + V_0\psi(x) = E\psi(x)$$

Since this is obviously satisfied, we have verified that (6-18) is a solution. Since it contains two arbitrary constants, it is the *general* solution to the time-independent Schroedinger equation for the region of the step potential where $V(x) = V_0$, with $E < V_0$. Although the increasing exponential part will not actually be used in the present section, it will be used in a subsequent section.

The arbitrary constants A, B, C, and D of (6-14) and (6-18) must be so chosen that the total eigenfunction satisfies the requirements concerning finiteness, single valuedness, and continuity, of $\psi(x)$ and $d\psi(x)/dx$. Consider first the behavior of $\psi(x)$ as $x \to +\infty$. In this region of the x axis the general form of $\psi(x)$ is given by (6-18). Inspection shows that it will generally increase without limit as $x \to +\infty$, because of the presence of the first term, $Ce^{k_2 x}$. In order to prevent this, and keep $\psi(x)$ finite, we must set the arbitrary coefficient C of the first term equal to zero. Thus we find

$$C = 0 \qquad (6\text{-}19)$$

Single valuedness is satisfied automatically by these functions. To study their continuity, we consider the point $x = 0$. At this point the two forms of $\psi(x)$, given by (6-14) and (6-18), must join in such a way that $\psi(x)$ and $d\psi(x)/dx$ are continuous. Continuity of $\psi(x)$ is obtained by satisfying the relation

$$D(e^{-k_2 x})_{x=0} = A(e^{ik_1 x})_{x=0} + B(e^{-ik_1 x})_{x=0}$$

which comes from equating the two forms at $x = 0$. This relation yields

$$D = A + B \qquad (6\text{-}20)$$

Continuity of the derivative of the two forms

$$\frac{d\psi(x)}{dx} = -k_2 De^{-k_2 x} \qquad x > 0$$

and

$$\frac{d\psi(x)}{dx} = ik_1 Ae^{ik_1 x} - ik_1 Be^{-ik_1 x} \qquad x < 0$$

is obtained by equating these derivatives at $x = 0$. Thus we set

$$-k_2 D(e^{-k_2 x})_{x=0} = ik_1 A(e^{ik_1 x})_{x=0} - ik_1 B(e^{-ik_1 x})_{x=0}$$

This yields

$$\frac{ik_2}{k_1} D = A - B \tag{6-21}$$

Adding (6-20) and (6-21) gives

$$A = \frac{D}{2}\left(1 + \frac{ik_2}{k_1}\right) \tag{6-22}$$

Subtracting gives

$$B = \frac{D}{2}\left(1 - \frac{ik_2}{k_1}\right) \tag{6-23}$$

We have now determined A, B, and C in terms of D. Thus the eigenfunction for the step potential, and for the energy $E < V_0$, is

$$\psi(x) = \begin{cases} \frac{D}{2}(1 + ik_2/k_1)e^{ik_1 x} + \frac{D}{2}(1 - ik_2/k_1)e^{-ik_1 x} & x \leq 0 \\ De^{-k_2 x} & x \geq 0 \end{cases} \tag{6-24}$$

The one remaining arbitrary constant, D, determines the amplitude of the eigenfunction, but it is not involved in any of its more important characteristics. The presence of this constant reflects the fact that the time-independent Schroedinger equation is linear in $\psi(x)$, and so solutions of any amplitude are allowed by the equation. We shall see that useful results can be usually obtained without bothering to carry through the normalization procedure that would specify D. The reason is that the measurable quantities that we shall obtain as predictions of the theory contain D in both the numerator and the denominator of a ratio, and so it cancels out.

The wave function corresponding to the eigenfunction is

$$\Psi(x,t) = \begin{cases} Ae^{ik_1 x}e^{-iEt/\hbar} + Be^{-ik_1 x}e^{-iEt/\hbar} = Ae^{i(k_1 x - Et/\hbar)} + Be^{i(-k_1 x - Et/\hbar)} & x \leq 0 \\ De^{-k_2 x}e^{-iEt/\hbar} & x \geq 0 \end{cases} \tag{6-25}$$

Consider the region $x < 0$. The first term in the wave function for this region is a traveling wave propagating in the direction of increasing x. This term describes a particle moving in the direction of increasing x. The second term in the wave function for $x < 0$ is a traveling wave propagating in the direction of decreasing x, and it describes a particle moving in that direction. This information, plus the classical predictions described earlier, suggests that we should associate the first term with the incidence of the particle on the potential step and the second term with the reflection of the particle from the step. Let us use this association to calculate the probability that the incident particle is reflected, which we call the *reflection coefficient* R. Obviously, R depends on the ratio B/A, which specifies the amplitude of the reflected part of the wave function relative to the amplitude of the incident part. But in quantum mechanics probabilities depend on intensities, such as B^*B and A^*A, not on

amplitudes. Thus, we must evaluate R from the formula

$$R = \frac{B^*B}{A^*A} \tag{6-26}$$

That is, the reflection coefficient is equal to the ratio of the intensity of the part of the wave that describes the reflected particle to the intensity of the part that describes the incident particle. We obtain

$$R = \frac{B^*B}{A^*A} = \frac{(1 - ik_2/k_1)^*(1 - ik_2/k_1)}{(1 + ik_2/k_1)^*(1 + ik_2/k_1)}$$

or

$$R = \frac{(1 + ik_2/k_1)(1 - ik_2/k_1)}{(1 - ik_2/k_1)(1 + ik_2/k_1)} = 1 \qquad E < V_0 \tag{6-27}$$

The fact that this ratio equals one means that a particle incident upon the potential step, with total energy less than the height of the step, has probability one of being reflected—it is always reflected. This is in agreement with the predictions of classical mechanics.

Consider now the eigenfunction of (6-24). Using the relation

$$e^{ik_1x} = \cos k_1x + i \sin k_1x \tag{6-28}$$

it is easy to show that the eigenfunction can be expressed as

$$\psi(x) = \begin{cases} D \cos k_1x - D\dfrac{k_2}{k_1} \sin k_1x & x \leq 0 \\ De^{-k_2x} & x \geq 0 \end{cases} \tag{6-29}$$

If we generate the wave function by multiplying $\psi(x)$ by $e^{-iEt/\hbar}$, we see immediately that we actually have a standing wave because the locations of the nodes do not change in time. In this problem the incident and reflected traveling waves for $x < 0$ combine to form a standing wave because they are of equal intensity. Figure 6-6 illustrates this schematically.

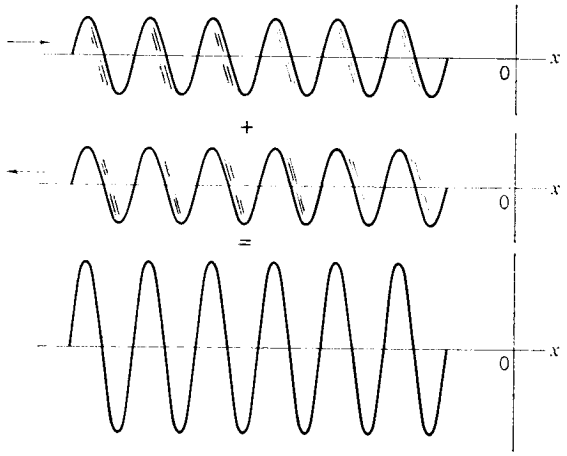


FIGURE 6-6

Illustrating schematically the combination of an incident and a reflected wave of equal intensities to form a standing wave. The wave function is reflected from a potential step at $x = 0$. Note that the nodes of the traveling waves move to the right or left, but those of the standing wave are stationary.

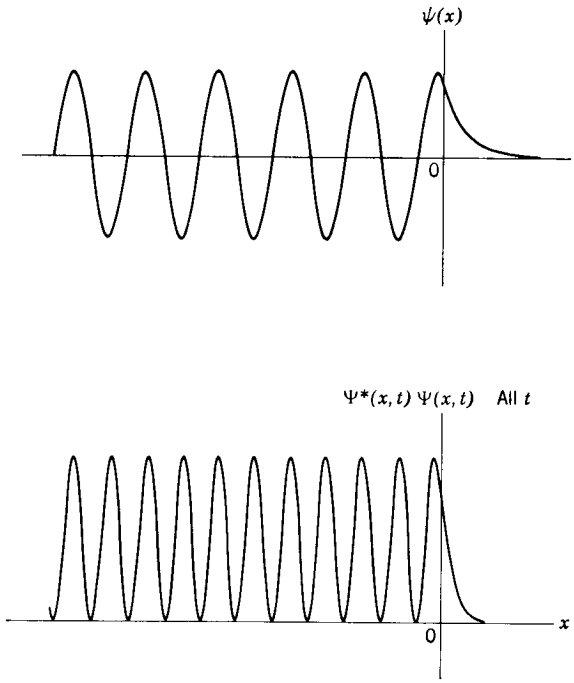


FIGURE 6-7

Top: The eigenfunction $\psi(x)$ for a particle incident upon a potential step at $x = 0$, with total energy less than the height of the step. Note the penetration of the eigenfunction into the classically excluded region $x > 0$. *Bottom:* The probability density $\Psi^*\Psi = \psi^*\psi = \psi^2$ corresponding to this eigenfunction. The spacing between the peaks of ψ^2 is twice as close as the spacing between the peaks of ψ.

In the top part of Figure 6-7 we illustrate the wave function by plotting the eigenfunction, (6-29), which is a real function of x if we take D real. The wave function can be thought of as oscillating in time according to $e^{-iEt/\hbar}$, with an amplitude whose space dependence is given by $\psi(x)$. Here we find a feature which is in sharp contrast to the classical predictions. Although in the region $x > 0$ the probability density

$$\Psi^*\Psi = D^*e^{-k_2x}e^{+iEt/\hbar}De^{-k_2x}e^{-iEt/\hbar} = D^*De^{-2k_2x} \tag{6-30}$$

illustrated in the bottom of Figure 6-7, decreases rapidly with increasing x, there *is* a finite probability of finding the particle in the region $x > 0$. In classical mechanics it would be absolutely impossible to find the particle in the region $x > 0$ because there the total energy is less than the potential energy, so the kinetic energy $p^2/2m$ is negative and the momentum p is imaginary. This phenomena, called *penetration of the classically excluded region*, is one of the more striking predictions of quantum mechanics.

We shall discuss later certain experiments which confirm this prediction, but here we should like to make several points about it. One is that penetration does *not* mean that the particle is stored in the classically excluded region. Indeed, we have seen that the incident particle is definitely reflected from the step.

Another point is that penetration of the excluded region, which obeys (6-30), is *not* in conflict with the experiments of classical mechanics. It is apparent from the equation that the probability of finding the particle with a coordinate $x > 0$ is only appreciable in a region starting at $x = 0$ and extending in a *penetration distance* Δx,

which equals $1/k_2$. The reason is that e^{-2k_2x} goes very rapidly to zero when x is very much larger than $1/k_2$. Since $k_2 = \sqrt{2m(V_0 - E)}/\hbar$, we have

$$\Delta x = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$$

In the classical limit, the product of m and $(V_0 - E)$ is so large, compared to $\hbar^2$, that Δx is immeasurably small.

Example 6-1. Estimate the penetration distance Δx for a very small dust particle, of radius $r = 10^{-6}$ m and density $\rho = 10^4$ kg/m^3, moving at the very low velocity $v = 10^{-2}$ m/sec, if the particle impinges on a potential step of height equal to twice its kinetic energy in the region to the left of the step.

The mass of the particle is

$$m = \frac{4}{3}\pi r^3 \rho \simeq 4 \times 10^{-18}\,\text{m}^3 \times 10^4\,\text{kg/m}^3 = 4 \times 10^{-14}\,\text{kg}$$

Its kinetic energy before hitting the step is

$$\frac{1}{2}mv^2 \simeq \frac{1}{2} \times 4 \times 10^{-14}\,\text{kg} \times 10^{-4}\,\text{m}^2/\text{sec}^2 = 2 \times 10^{-18}\,\text{joule}$$

and this is also the value of $(V_0 - E)$. The penetration distance is

$$\Delta x = \frac{\hbar}{\sqrt{2m(V_0 - E)}} \simeq \frac{10^{-34}\,\text{joule-sec}}{\sqrt{2 \times 4 \times 10^{-14}\,\text{kg} \times 2 \times 10^{-18}\,\text{joule}}}$$
$$\simeq 2 \times 10^{-19}\,\text{m}$$

Of course, this is many orders of magnitude smaller than could be detected in any possible measurement. For the more massive particles and higher energies typically considered in classical mechanics, Δx is even smaller. ◀

Furthermore, we should like to point out that the uncertainty principle shows the wavelike properties exhibited by an entity in penetrating the classically excluded region are really *not* in conflict with its particlelike properties. Consider an experiment capable of proving that the particle is located somewhere in the region $x > 0$. Since the probability density for $x > 0$ is appreciable only in a range of length Δx, the experiment amounts to localizing the particle within that range. In doing this, the experiment necessarily leads to an uncertainty Δp in the momentum, which must be at least as large as

$$\Delta p \simeq \frac{\hbar}{\Delta x} \simeq \sqrt{2m(V_0 - E)}$$

Consequently, the energy of the particle is uncertain by an amount

$$\Delta E \simeq \frac{(\Delta p)^2}{2m} \simeq V_0 - E$$

and it is no longer possible to say that the total energy E of the particle is definitely less than the potential energy V_0. This removes the conflict alluded to.

Penetration of the classically excluded region *can* lead to measurable consequences. We shall see this later for a potential that steps up to a height $V_0 > E$, but remains up only for a distance not much larger than the penetration distance Δx, and then steps down. In fact, the phenomenon has significant practical consequences. One example, which we shall refer to soon, is the tunnel diode used in modern electronics.

Example 6-2. A conduction electron moves through a block of Cu at total energy E under the influence of a potential which, to a good approximation, has a constant value of zero in the interior of the block and abruptly steps up to the constant value $V_0 > E$ outside the block. The interior value of the potential is essentially constant, at a value that can be taken as zero, since a conduction electron inside the metal feels little net Coulomb force exerted by the approximately uniform charge distributions that surround it. The potential increases very rapidly at the surface of the metal, to its exterior value V_0, because there the electron feels a strong force exerted by the nonuniform charge distributions present in that region. This force tends to attract the electron back into the metal and is, of course, what causes the conduction electron to be bound to the metal. Because the electron is bound, V_0 must be greater than its total energy E. The exterior value of the potential is constant, if the metal has no total charge, since outside the metal the electron would feel no force at all. The mass of the electron is $m = 9 \times 10^{-31}$ kg. Measurements of the energy required to permanently remove it from the block, i.e., measurements of the work function, show that $V_0 - E = 4$ eV. From these data estimate the distance Δx that the electron can penetrate into the classically excluded region outside the block.

In the mks system

$$V_0 - E = 4 \text{ eV} \times \frac{1.6 \times 10^{-19} \text{ joule}}{1 \text{ eV}} \simeq 6 \times 10^{-19} \text{ joule}$$

So

$$\Delta x = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$$

$$\simeq \frac{10^{-34} \text{ joule-sec}}{\sqrt{2 \times 9 \times 10^{-31} \text{ kg} \times 6 \times 10^{-19} \text{ joule}}} \simeq 10^{-10} \text{ m}$$

The penetration distance is of the order of atomic dimensions. Therefore, the effect can be of consequence in atomic systems. We shall find soon that, in certain circumstances, the effect is very important indeed. ◀

Let us finally make the point that penetration of the classically excluded region is nonclassical in the sense that an entity that does it is not behaving like a classical *particle*. But it is behaving like a classical *wave* since, as we shall see later, the phenomenon has been known to occur with light waves since the time of Newton. Penetration of the classically excluded region by material particles is just another manifestation of the wavelike nature of material particles.

Figure 6-8 shows the probability density for a wave function in the form of a *group*, for the problem of a particle incident in the direction of increasing x upon a potential step with an average value of the total energy less than the step height. The wave function can be obtained by summing, over the total energy E, a very large number of wave functions of the form we have obtained in (6-25). It can also be obtained by a direct numerical solution of the Schroedinger equation. Either way involves a large amount of work on a high-speed computer, as can be guessed from the complications indicated in the figure. The results of the calculations certainly convey a realistic sense of the particle motion; but note that these results show, again, that the particle associated with the wave function is reflected from the step with probability one, and that there is some penetration of the classically excluded region. The fact that we have been able to learn these basic results from simple calculations, involving only the wave function of (6-25) which contains a single value of E, is an example of the fact that it is generally not necessary in quantum mechanics to use wave functions in the form of groups. Of course, we must be willing to learn how to interpret the simple wave functions.

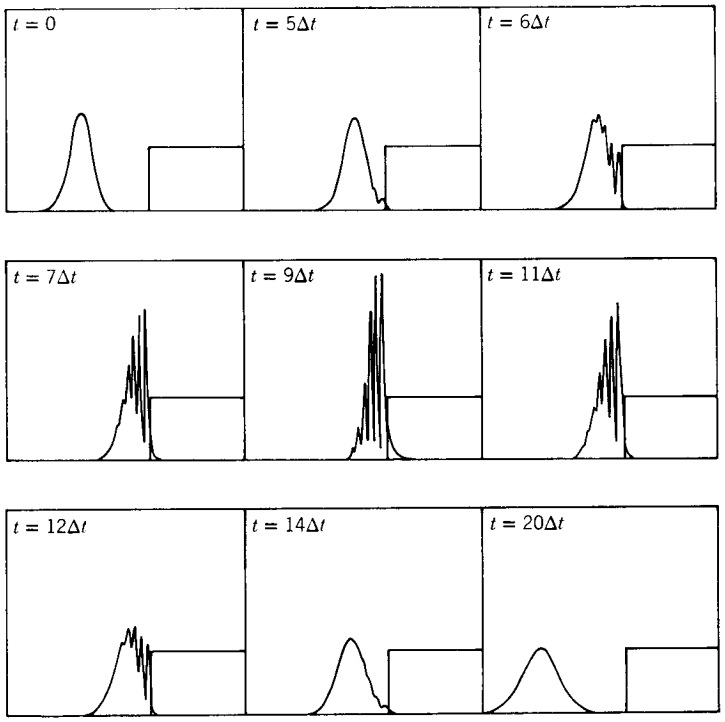


FIGURE 6-8

A potential step, and the probability density $\Psi^*\Psi$ for a group wave function describing a particle incident on the step with total energy less than the step height. As time evolves, the group moves up to the step, penetrates slightly into the classically excluded region, and then is completely reflected from the step. The complications of the mathematical treatment using a group are indicated by the complications of its structure during reflection.

6-4 The Step Potential (Energy Greater Than Step Height)

In this section we consider the motion of a particle under the influence of a step potential, (6-11), when its total energy E is greater than the height V_0 of the step. That is, we take $E > V_0$, as illustrated in Figure 6-9.

In *classical mechanics*, a particle of total energy E traveling in the region $x < 0$, in the direction of increasing x, will suffer an impulsive retarding force $F = -dV(x)/dx$ at the point $x = 0$. But the impulse will only slow the particle, and it will enter the region $x > 0$, continuing its motion in the direction of increasing x. Its total energy E

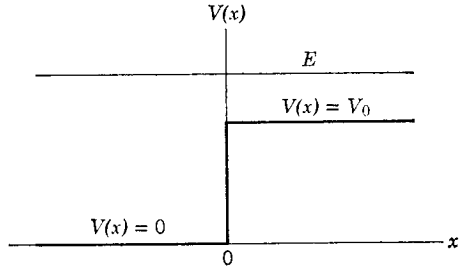


FIGURE 6-9

The relation between total and potential energies for a particle incident upon a potential step with total energy greater than the height of the step.

remains constant; its momentum in the region $x < 0$ is p_1, where $p_1^2/2m = E$; its momentum in the region $x > 0$ is p_2, where $p_2^2/2m = E - V_0$.

We shall see that the predictions of *quantum mechanics* are not so simple. If E is not too much larger than V_0, the theory predicts that the particle has an appreciable chance of being reflected at the step back into the region $x < 0$, even though it has enough energy to pass over the step into the region $x > 0$.

One example of this is found in the case of an electron in the cathode of a photoelectric cell, which has received energy from absorbing a photon, and which is trying to escape the surface of the metallic cathode. If its energy is not much higher than the height of the step in the potential that it feels at the surface of the metal, it may be reflected back and not succeed in escaping. This leads to a significant reduction in the efficiency of photocells for light of frequencies not far above the cutoff frequency.

A more important example of reflection occurring when a particle tries to pass over a potential step is found in the motion of a neutron in a nucleus. To a good approximation, the potential acting on the neutron near the nuclear surface is a step potential. The potential rises very rapidly at the nuclear surface because a nucleus tends to bind a neutron. If the neutron has received energy, in one way or another, and is trying to escape the nucleus, it will probably be reflected back into the nucleus at the surface if its energy is only a little greater than the step height. This has the effect of inhibiting the emission of lower energy neutrons from nuclei, and thereby considerably increases the stability of nuclei in low-lying excited states. The effect is a manifestation of the wavelike properties of neutrons that is very significant in the processes taking place in nuclear reactions, as we shall see near the end of this book.

In quantum mechanics, the motion of the particle under the influence of the step potential is described by the wave function

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$$

where the eigenfunction $\psi(x)$ satisfies the time-independent Schroedinger equation for the potential. This equation has different forms in the regions to the left and right of the potential step, namely

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \qquad x < 0 \quad (6\text{-}31)$$

and

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = (E - V_0)\psi(x) \qquad x > 0 \quad (6\text{-}32)$$

The eigenfunction $\psi(x)$ also satisfies the conditions requiring finiteness, single valuedness, and continuity, for it and its derivative, particularly at the joining point $x = 0$.

Equation (6-31) describes the motion of a free particle of momentum p_1. Its general solution is

$$\psi(x) = Ae^{ik_1x} + Be^{-ik_1x} \qquad x < 0 \quad (6\text{-}33)$$

where

$$k_1 = \frac{\sqrt{2mE}}{\hbar} = \frac{p_1}{\hbar}$$

Equation (6-32) describes the motion of a free particle of momentum p_2. Its general solution is

$$\psi(x) = Ce^{ik_2x} + De^{-ik_2x} \qquad x > 0 \quad (6\text{-}34)$$

where

$$k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar} = \frac{p_2}{\hbar} \qquad E > V_0$$

The wave function specified by these two forms consists of traveling waves of de Broglie wavelength $\lambda_1 = h/p_1 = 2\pi/k_1$ in the region $x < 0$, and of longer de Broglie wavelength $\lambda_2 = h/p_2 = 2\pi/k_2$ in the region $x > 0$. Note that the functions we deal with here already satisfy the requirements of finiteness and single valuedness; but we must explicitly consider their continuity, and we shall do so shortly.

A particle initially in the region $x < 0$, and moving towards $x = 0$ would, in classical mechanics, have probability one of passing the point $x = 0$ and entering the region $x > 0$. This is not true in quantum mechanics. Because of the wavelike properties of the particle, there is a certain probability that the particle will be reflected at the point $x = 0$, where there is a discontinuous change in the de Broglie wavelength. Thus we need to take both terms of the general solution of (6-33) to describe the incident and reflected traveling waves in the region $x < 0$. We do not, however, need to take the second term of the general solution of (6-34). This term describes a wave traveling in the direction of decreasing x in the region $x > 0$. Since the particle is incident in the direction of increasing x, such a wave could arise only from a reflection at some point with a large positive x coordinate (well beyond the discontinuity at $x = 0$). As there is nothing out there to cause a reflection, we know that there is only a transmitted traveling wave in the region $x > 0$, and so we set the arbitrary constant

$$D = 0 \tag{6-35}$$

The arbitrary constants A, B, and C must be chosen to make $\psi(x)$ and $d\psi(x)/dx$ continuous at $x = 0$. The first requirement, that the values of $\psi(x)$ expressed by (6-33) and (6-34) be the same at $x = 0$, is satisfied if

$$A(e^{ik_1x})_{x=0} + B(e^{-ik_1x})_{x=0} = C(e^{ik_2x})_{x=0}$$

or

$$A + B = C \tag{6-36}$$

The second requirement, that the values of the derivatives of the two expressions for $\psi(x)$ be the same at $x = 0$, is satisfied if

$$ik_1A(e^{ik_1x})_{x=0} - ik_1B(e^{-ik_1x})_{x=0} = ik_2C(e^{ik_2x})_{x=0}$$

or

$$k_1(A - B) = k_2C \tag{6-37}$$

From the last two numbered equations, we find

$$B = \frac{k_1 - k_2}{k_1 + k_2}A \qquad \text{and} \qquad C = \frac{2k_1}{k_1 + k_2}A \tag{6-38}$$

Thus the eigenfunction is

$$\psi(x) = \begin{cases} Ae^{ik_1x} + A\dfrac{k_1 - k_2}{k_1 + k_2}e^{-ik_1x} & x \leq 0 \\ A\dfrac{2k_1}{k_1 + k_2}e^{ik_2x} & x \geq 0 \end{cases} \tag{6-39}$$

As before, it will not be necessary to evaluate the arbitrary constant A that determines the amplitude of the eigenfunction.

It is clear that an eigenfunction satisfying the two continuity conditions could not have been found if we had initially set the coefficient B of the reflected wave equal to zero. We would then

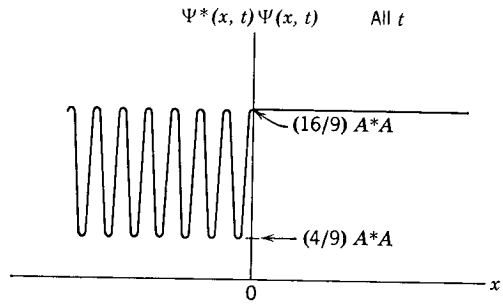


FIGURE 6-10
The probability density $\Psi^*\Psi$ for the eigenfunction of (6-39), when $k_1 = 2k_2$.

have had only two arbitrary constants to satisfy the two continuity conditions, and we would not have had one left over to play the role, demanded by the linearity of the time-independent Schroedinger equation, of an arbitrary constant that determines the amplitude of the eigenfunction.

By analogy with our interpretation of the eigenfunction of (6-24), we recognize that the first term in the expression of (6-39) valid for $x < 0$ (left of the discontinuity) represents the incident traveling wave; the second term in the expression valid for $x < 0$ represents the reflected traveling wave; and the expression valid for $x > 0$ (right of the discontinuity) represents the transmitted traveling wave.

Figure 6-10 illustrates the probability density $\Psi^*(x,t)\Psi(x,t) = \psi^*(x)\psi(x)$ for the wave function $\Psi(x,t)$ corresponding to the eigenfunction $\psi(x)$ of (6-39) (in the representative case $k_1 = 2k_2$). We do not plot either the eigenfunction or wave function as both are complex. In the region $x > 0$ the wave function is a pure traveling wave (of amplitude $4A/3$ in this case) traveling to the right, and so the probability density is constant as in the bottom part of Figure 6-1. In the region $x < 0$ the wave function is a combination of the incident traveling wave (of amplitude A) moving to the right, and a reflected traveling wave (of amplitude $A/3$) moving to the left. As the amplitude of the reflected wave is necessarily smaller than that of the incident wave, the two cannot combine to yield a pure standing wave. Their sum $\Psi(x,t)$ in that region is, instead, something between a standing wave and a traveling wave. This is seen in the behavior of $\Psi^*(x,t)\Psi(x,t)$ for $x < 0$, which looks like something between the pure standing wave probability density of Figure 6-7 and the pure traveling wave probability density of Figure 6-1 in that it oscillates but has minimum values greater than zero.

The ratio of the intensity of the reflected wave to the intensity of the incident wave gives the probability that the particle will be reflected by the potential step back into the region $x < 0$. This probability is the *reflection coefficient* R. That is

$$R = \frac{B^*B}{A^*A} = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^*\left(\frac{k_1 - k_2}{k_1 + k_2}\right) = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 \qquad E > V_0 \quad (6\text{-}40)$$

We see from this result that $R < 1$ when $E > V_0$, i.e., when the total energy of the particle is greater than the height of the potential step. This is in contrast to the value $R = 1$ when $E < V_0$, that we obtained from the result of Section 6-3. Of course, the thing that is surprising about the present result is not that $R < 1$, but that $R > 0$. It is surprising because a classical particle would definitely not be reflected if it had enough energy to pass the potential discontinuity. On the other hand, at a corresponding discontinuity a classical wave would be reflected, as we shall discuss shortly.

Also of interest is the *transmission coefficient* T, which specifies the probability that the particle will be transmitted past the potential step from the region $x < 0$ into the region $x > 0$. The evaluation of T is slightly more complicated than the evaluation

of R because the velocity of the particle is different in the two regions. According to accepted convention, transmission and reflection coefficients are actually defined in terms of the ratios of probability fluxes. A *probability flux* is the probability per second that a particle will be found crossing some reference point traveling in a particular direction. The incident probability flux is the probability per second of finding a particle crossing a point at $x < 0$ in the direction of increasing x; the reflected probability flux is the probability per second of finding a particle crossing a point at $x < 0$ in the direction of decreasing x; and the transmitted probability flux is the probability per second of finding a particle crossing a point at $x > 0$ in the direction of increasing x. Since the probability per second that a particle will cross a given point is proportional to the distance it travels per second, the probability flux is proportional not only to the intensity of the appropriate wave but also to the appropriate velocity of the particle. Thus, according to the strict definition, the reflection coefficient R is

$$R = \frac{v_1 B^* B}{v_1 A^* A} = \frac{B^* B}{A^* A} \tag{6-41}$$

where v_1 is the velocity of the particle in the region $x < 0$. Since the velocities cancel, what remains is identical to the formula we have used previously for R. For T, the velocities do *not* cancel, and we have

$$T = \frac{v_2 C^* C}{v_1 A^* A} = \frac{v_2}{v_1}\left(\frac{2k_1}{k_1 + k_2}\right)^2$$

where v_2 is the velocity of the particle in the region $x > 0$. Now

$$v_1 = \frac{p_1}{m} = \frac{\hbar k_1}{m} \qquad \text{and} \qquad v_2 = \frac{p_2}{m} = \frac{\hbar k_2}{m}$$

So the above expression gives

$$T = \frac{k_2}{k_1}\frac{(2k_1)^2}{(k_1 + k_2)^2} = \frac{4k_1 k_2}{(k_1 + k_2)^2} \qquad E > V_0 \tag{6-42}$$

It is easy to show by evaluating R and T from (6-40) and (6-42) that

$$R + T = 1 \tag{6-43}$$

This useful relation is the motivation for defining the reflection and transmission coefficients in terms of probability fluxes.

The probability flux incident upon the potential step is split into a transmitted flux and a reflected flux. But (6-43) says their sum equals the incident flux; i.e., the probability that the particle is either transmitted *or* reflected is one. The particle does not vanish at the step; nor does the particle itself split at the step. In any particular trial the particle will go one way or the other. For a large number of trials, the average probability of going in the direction of decreasing x is measured by R, and the average probability of going in the direction of increasing x is measured by T.

Note that R and T are both unchanged in value if k_1 and k_2 are exchanged in (6-40) and (6-42). A moment's consideration should convince the student that this means the same values of R and T would be obtained if the particle were incident upon the potential step in the direction of decreasing x from the region $x > 0$. The wave function describing the motion of the particle, and consequently the probability flux, is partially reflected simply because there is a discontinuous change in $V(x)$, and not because $V(x)$ becomes larger in the direction of the incidence of the particle. The behavior of R and T when k_1 and k_2 are exchanged involves a characteristic property

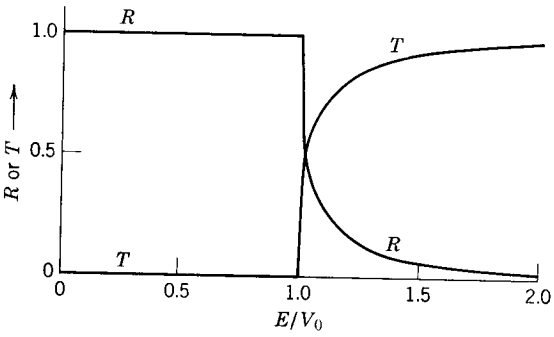


FIGURE 6-11

The reflection and transmission coefficients R and T for a particle incident upon a potential step. The abscissa E/V_0 is the ratio of the total energy of the particle to the increase in its potential energy at the step. The case $k_1 = 2k_2$, illustrated in Figure 6-10, corresponds to $E/V_0 = 1.33$.

of all waves that, in optics, is sometimes called the *reciprocity* property. When light passes perpendicularly through a sharp interface between media with different indices of refraction, a fraction of the light is reflected because of the abrupt change in its wavelength, and the same fraction is reflected independent of whether it is incident from one side of the interface or from the other. Exactly the same thing happens when a microscopic particle experiences an abrupt change in its de Broglie wavelength. In fact, the equations governing the two phenomena are identical in form. We see, once again, that a microscopic particle moves in a wavelike manner.

In Figure 6-11 the reflection and transmission coefficients are plotted as a function of the convenient ratio E/V_0. By evaluating k_1 and k_2 in (6-40) and (6-42), we find that these expressions for the reflection and transmission coefficients can be written in terms of the ratio as

$$R = 1 - T = \left(\frac{1 - \sqrt{1 - V_0/E}}{1 + \sqrt{1 - V_0/E}}\right)^2 \qquad \frac{E}{V_0} > 1 \quad (6\text{-}44)$$

The figure also plots the results

$$R = 1 - T = 1 \qquad \frac{E}{V_0} < 1$$

obtained in (6-27) of the preceding section for a step potential when $E/V_0 < 1$.

As an example, for $E/V_0 = 1.33$ the transmission coefficient has the value $T = 0.88$. This E/V_0 ratio corresponds to the case $k_2 = k_1/2$ whose probability density pattern is illustrated in Figure 6-10. Note from that figure that the probability of finding the particle in a given length of the x axis, which is long enough to average over the quantum mechanical fluctuations in the probability density, is nearly twice as large to the right of the potential step as it is to the left of the step. From a classical point of view, which is appropriate to discussing an average over quantum mechanical fluctuations, it can be said that the reasons for this are: (a) the probability that the particle will pass the step and proceed into the region to its right is almost equal to one, and (b) the particle's velocity is halved when it enters the region to the right of the step since $k = p/\hbar = mv/\hbar$ and $k_2 = k_1/2$, so it spends twice as much time in any given length of the axis in that region.

From Figure 6-11 we see that the energy of the particle must be appreciably higher than the height of the potential step before the probability of reflection becomes negligible. However, the case in which E becomes very large is not necessarily the case of the classical limit for which we know there will be no reflection at all. The point is that (6-44) says R depends only on the ratio E/V_0, so that it will keep the same value if V_0 increases as rapidly as E. This seems paradoxical until we realize that, in the limit of large energies, our basic assumption that the change in the value of the step potential $V(x)$ is perfectly sharp can no longer be even an approximation to a real

physical situation. If the potential function changes only very gradually with x, then the de Broglie wavelength will change only very gradually. In this case the reflection will be negligible because the change in wavelength is gradual, and reflection arises from an abrupt change in the wavelength. Specifically, if the fractional change in $V(x)$ is very small when x changes by one de Broglie wavelength, then the reflection coefficient will be very small. This gives rise to the classical limit since in that limit the de Broglie wavelength is so short that any physically realistic potential $V(x)$ changes only by a negligible fraction in one wavelength.

For particles in atomic or nuclear systems, the de Broglie wavelength can be long relative to the distance in which the potential experienced by the particle changes value significantly. Then the step potential is a very good approximation. For these microscopic particles, the probability of reflection can be large.

Example 6-3. When a neutron enters a nucleus, it experiences a potential energy which drops at the nuclear surface very rapidly from a constant external value $V = 0$ to a constant internal value of about $V = -50$ MeV. The decrease in the potential is what makes it possible for a neutron to be bound in a nucleus. Consider a neutron incident upon a nucleus with an external kinetic energy $K = 5$ MeV, which is typical for a neutron that has just been emitted from a nuclear fission. Estimate the probability that the neutron will be reflected at the nuclear surface, thereby failing to enter and have its chance at inducing another nuclear fission.

For an estimate, we may take the neutron-nucleus potential to be a one-dimensional step potential, as illustrated in Figure 6-12. Because of the reciprocity property of the reflection coefficient, we may evaluate it from (6-44), using $V_0 = 50$ MeV and $E = 55$ MeV for reasons that can be seen by inspection of the figure. We have

$$R = \left(\frac{1 - \sqrt{1 - 50/55}}{1 + \sqrt{1 - 50/55}}\right)^2 \simeq 0.29$$

This estimate gives a correct impression of the great importance of the reflection phenomenon when low energy neutrons collide with nuclei. But the numerical value we have obtained for the reflection coefficient is not very accurate since the actual neutron-nucleus potential does not drop quite as rapidly at the nuclear surface, in comparison to the de Broglie wavelength, as a step potential. ◀

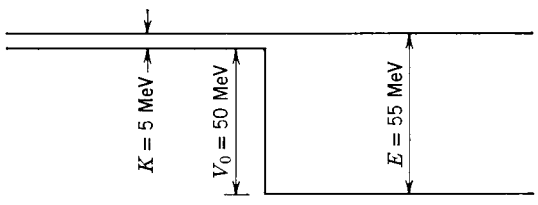
6-5 The Barrier Potential

In this section we consider a *barrier potential*, illustrated in Figure 6-13. The potential can be written as follows

$$V(x) = \begin{cases} V_0 & 0 < x < a \\ 0 & x < 0 \text{ or } x > a \end{cases} \tag{6-45}$$

FIGURE 6-12

A neutron of external kinetic energy K incident upon a decreasing potential step of depth V_0, which approximates the potential it feels upon entering a nucleus. Its total energy, measured from the bottom of the step potential, is E.



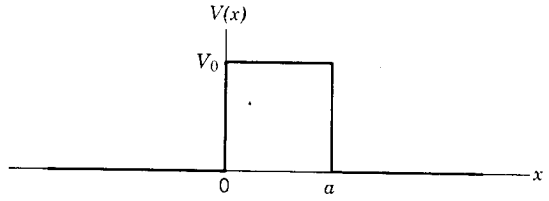


FIGURE 6-13
A barrier potential.

According to *classical mechanics*, a particle of total energy E in the region $x < 0$, which is incident upon the barrier in the direction of increasing x, will have probability one of being reflected if $E < V_0$, and probability one of being transmitted into the region $x > a$ if $E > V_0$.

Neither of these statements describes accurately the *quantum mechanical* results. If E is not much larger than V_0, the theory predicts that there will be some reflection, except for certain values of E. If E is not much smaller than V_0, quantum mechanics predicts that there is a certain probability that the particle will be transmitted through the barrier into the region $x > a$.

In "tunneling" through a barrier whose height exceeds its total energy, a material particle is behaving purely like a wave. But in the region beyond the barrier it can be detected as a localized particle, without introducing a significant uncertainty in the knowledge of its energy. Thus penetration of a classically excluded region of limited width by a particle *can* be observed, in the sense that the particle can be observed to be a particle, of total energy less than the potential energy in the excluded region, both before and after it penetrates the region. We shall discuss some consequences of this fascinating effect in the present section, as well as some consequences of the reflection of particles attempting to pass over a barrier. The following section is devoted completely to examples of tunneling through barriers, and considers three of particular importance: (1) the emission of α particles from radioactive nuclei through the potential barrier they experience in the vicinity of the nuclei, (2) the inversion of the ammonia molecule which provides a frequency standard for atomic clocks, and (3) the tunnel diode used as a switching unit in fast electronic circuits.

For the barrier potential of (6-45), we know from the qualitative arguments of the last chapter that acceptable solutions to the time-independent Schroedinger equation should exist for *all* values of the total energy $E \geq 0$. We also know that the equation breaks up into three separate equations for the three regions: $x < 0$ (left of the barrier), $0 < x < a$ (within the barrier), and $x > a$ (right of the barrier). In the regions to the left and to the right of the barrier the equations are those for a free particle of total energy E. Their general solutions are

$$\begin{aligned} \psi(x) &= Ae^{ik_{\mathrm{I}}x} + Be^{-ik_{\mathrm{I}}x} && x < 0 \\ \psi(x) &= Ce^{ik_{\mathrm{I}}x} + De^{-ik_{\mathrm{I}}x} && x > a \end{aligned} \tag{6-46}$$

where

$$k_{\mathrm{I}} = \frac{\sqrt{2mE}}{\hbar}$$

In the region within the barrier, the form of the equation, and of its general solution, depends on whether $E < V_0$ or $E > V_0$. Both of these cases have been treated in the previous sections. In the first case, $E < V_0$, the general solution is

$$\psi(x) = Fe^{-k_{\mathrm{II}}x} + Ge^{k_{\mathrm{II}}x} \qquad 0 < x < a \tag{6-47}$$

where

$$k_{\mathrm{II}} = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \qquad E < V_0$$

In the second case, $E > V_0$, it is

$$\psi(x) = Fe^{ik_{III}x} + Ge^{-ik_{III}x} \qquad 0 < x < a \quad (6\text{-}48)$$

where

$$k_{III} = \frac{\sqrt{2m(E - V_0)}}{\hbar} \qquad E > V$$

Note that (6-47) involves *real* exponentials, whereas (6-46) and (6-48) involve *complex* exponentials.

Since we are considering the case of a particle incident on the barrier from the left, in the region to the right of the barrier there can be only a transmitted wave as there is nothing in that region to produce a reflection. Thus we can set

$$D = 0$$

In the present situation, however, we cannot set $G = 0$ in (6-47) since the value of x is limited in the barrier region, $0 < x < a$, so $\psi(x)$ for $E < V_0$ cannot become infinitely large even if the increasing exponential is present. Nor can we set $G = 0$ in (6-48) since $\psi(x)$ for $E > V_0$ will have a reflected component in the barrier region that arises from the potential discontinuity at $x = a$.

We consider first the case in which the energy of the particle is less than the height of the barrier, i.e., the case:

$E < V_0$

In matching $\psi(x)$ and $d\psi(x)/dx$ at the points $x = 0$ and $x = a$, four equations in the arbitrary constants A, B, C, F, and G will be obtained. These equations can be used to evaluate B, C, F, and G in terms of A. The value of A determines the amplitude of the eigenfunction, and it can be left arbitrary. The form of the probability density corresponding to the eigenfunction obtained is indicated in Figure 6-14 for a typical situation. In the region $x > a$ the wave function is a pure traveling wave and so the probability density is constant, as for $x > 0$ in Figure 6-10. In the region $x < 0$ the wave function is principally a standing wave but has a small traveling wave component because the reflected traveling wave has an amplitude less than that of the incident wave. So the probability density in that region oscillates but has minimum values somewhat greater than zero, as for $x < 0$ in Figure 6-10. In the region $0 < x < a$ the wave function has components of both types, but it is principally a standing wave of exponentially decreasing amplitude, and this behavior can be seen in the behavior of the probability density in the region.

The most interesting result of the calculation is the ratio T, of the probability flux transmitted through the barrier into the region $x > a$, to the probability flux incident

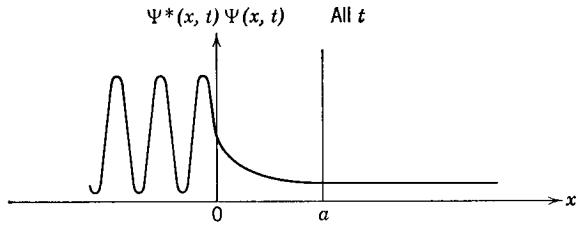


FIGURE 6-14

The probability density function $\Psi^*\Psi$ for a typical barrier penetration situation.

upon the barrier. This transmission coefficient is found to be

$$T = \frac{v_1 C^* C}{v_1 A^* A} = \left[1 + \frac{(e^{k_{II}a} - e^{-k_{II}a})^2}{16\dfrac{E}{V_0}\left(1 - \dfrac{E}{V_0}\right)}\right]^{-1} = \left[1 + \frac{\sinh^2 k_{II}a}{4\dfrac{E}{V_0}\left(1 - \dfrac{E}{V_0}\right)}\right]^{-1} \tag{6-49}$$

where

$$k_{II}a = \sqrt{\frac{2mV_0a^2}{\hbar^2}\left(1 - \frac{E}{V_0}\right)} \qquad E < V_0$$

If the exponents are very large, this formula reduces to

$$T \simeq 16\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)e^{-2k_{II}a} \qquad k_{II}a \gg 1 \tag{6-50}$$

as can be verified with ease. When (6-50) is a good approximation, T is extremely small.

These equations make a prediction which is, from the point of view of classical mechanics, very remarkable. They say that a particle of mass m and total energy E, incident on a potential barrier of height $V_0 > E$ and finite thickness a, actually has a certain probability T of penetrating the barrier and appearing on the other side. This phenomenon is called *barrier penetration*, and the particle is said to *tunnel* through the barrier. Of course, T is vanishingly small in the classical limit because in that limit the quantity $2mV_0a^2/\hbar^2$, which is a measure of the opacity of the barrier, is extremely large.

We shall discuss barrier penetration in detail shortly, but let us first finish describing the calculations by considering the case in which the energy of the particle is greater than the height of the barrier, i.e., the case:

$E > V_0$

In this case the eigenfunction is oscillatory in all three regions, but of longer wavelength in the barrier region, $0 < x < a$. Evaluation of the constants B, C, F, and G by application of the continuity conditions at $x = 0$ and $x = a$, leads to the following formula for the transmission coefficient

$$T = \frac{v_1 C^* C}{v_1 A^* A} = \left[1 - \frac{(e^{ik_{III}a} - e^{-ik_{III}a})^2}{16\dfrac{E}{V_0}\left(\dfrac{E}{V_0} - 1\right)}\right]^{-1} = \left[1 + \frac{\sin^2 k_{III}a}{4\dfrac{E}{V}\left(\dfrac{E}{V_0} - 1\right)}\right]^{-1} \tag{6-51}$$

where

$$k_{III}a = \sqrt{\frac{2mV_0a^2}{\hbar^2}\left(\frac{E}{V_0} - 1\right)} \qquad E > V_0$$

Example 6-4. An electron is incident upon a rectangular barrier of height $V_0 = 10$ eV and thickness $a = 1.8 \times 10^{-10}$ m. This rectangular barrier is an idealization of the barrier encountered by an electron that is scattering from a negatively ionized gas atom in the "plasma" of a gas discharge tube. The actual barrier is not rectangular, of course, but it is about the height and thickness quoted. Evaluate the transmission coefficient T and the reflection coefficient R, as a function of the total energy E of the electron.

From Example 6-2 we can see that if E is a reasonable fraction of V_0 the penetration length Δx will be comparable to the barrier thickness a. Thus we can expect appreciable transmission through the barrier. To determine exactly how much, we use the numbers given to evaluate

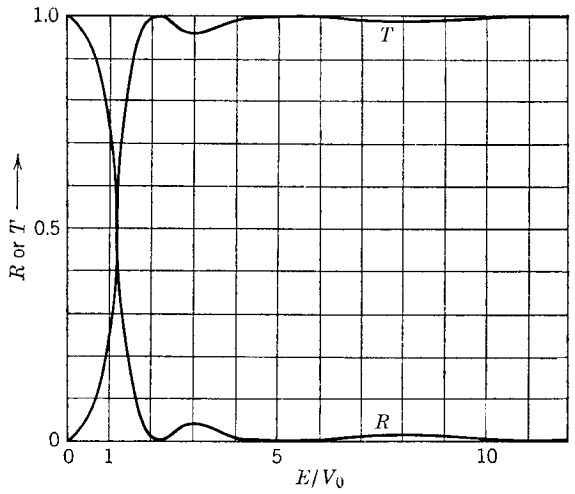


FIGURE 6-15

The reflection and transmission coefficients R and T for a particle incident upon a potential barrier of height V_0 and thickness a, such that $2mV_0a^2/\hbar^2 = 9$. The abscissa E/V_0 is the ratio of the total energy of the particle to the height of the potential barrier.

the combination of parameters

$$\frac{2mV_0a^2}{\hbar^2} \simeq \frac{2 \times 9 \times 10^{-31}\,\text{kg} \times 10\,\text{eV} \times 1.6 \times 10^{-19}\,\text{joule/eV} \times (1.8)^2 \times 10^{-20}\,\text{m}^2}{10^{-68}\,\text{joule}^2\text{-sec}^2} \simeq 9$$

which enters (6-49). From this we can plot T, and also $R = 1 - T$, versus E/V_0, in the range $0 \leq E/V_0 \leq 1$. The plot is shown in Figure 6-15. We see that T is very small when $E/V_0 \ll 1$. But, when E/V_0 is only somewhat smaller than one, so that E is nearly as large as V_0, T is not at all negligible. For instance, when E is half as large as V_0 so that $E/V_0 = 0.5$, the transmission coefficient has the appreciable value $T \simeq 0.05$. It is apparent that electrons can penetrate this barrier with relative ease.

For $E/V_0 > 1$, we evaluate T, and $R = 1 - T$, from (6-51), using the same combination of parameters as before. The results are also shown in Figure 6-15. For $E/V_0 > 1$, the transmission coefficient T is in general somewhat less than one, owing to reflection at the discontinuities in the potential. However, from (6-51) it can be seen that $T = 1$ whenever $k_{III}a = \pi, 2\pi, 3\pi, \ldots$. This is simply the condition that the length of the barrier region, a, is equal to an integral or half-integral number of de Broglie wavelengths $\lambda_{III} = 2\pi/k_{III}$ in that region. For this particular barrier, electrons of energy $E \simeq 21$ eV, 53 eV, etc., satisfy the condition $k_{III}a = \pi, 2\pi$, etc., and so pass into the region $x > a$ without any reflection. The effect is a result of constructive interference between reflections at $x = 0$ and $x = a$. It is closely related to the *Ramsauer effect* observed in the scattering of low-energy electrons by noble gas atoms, in which electrons of certain energies in the range of a few electron volts pass through these atoms as if they were not there, and so have transmission coefficients equal to one. Essentially the same effect is seen in scattering of neutrons, with energies of a few MeV, from all nuclei. The nuclear effect, called *size resonance*, will be discussed later in the book. ◀

We can bring together the results of the last three sections by comparing the plot of the energy dependence of the reflection coefficient R for a barrier potential, in Figure 6-15, with the plot of the same thing for a step potential, in Figure 6-11. The

comparison shows that for both potentials $R \to 1$ as $E/V_0 \to 0$, and $R \to 0$ as $E/V_0 \to \infty$, with the decrease in R occurring around $E/V_0 = 1$. But for the barrier potential the reflection coefficient approaches one gradually, at small energies, since the finite thickness of the classically excluded region allows some transmission. Also, the barrier potential reflection coefficient oscillates, at large energies, because of interferences in the reflections from its two discontinuities. As the step potential can be considered to be a limiting case of a barrier of very great width, we can see from our comparison the behavior of the barrier potential reflection coefficient in this limit.

Now we shall discuss in some detail the origins of these results. They all involve phenomena which arise from the wavelike behavior of the motion of microscopic particles, and each phenomenon is also observed in other types of wave motion. As we remarked in Chapter 5, the time-independent differential equation governing classical wave motion is of the same form as the time-independent Schroedinger equation. For instance, electromagnetic radiation of frequency ν propagating through a medium with index of refraction μ obeys the equation

$$\frac{d^2\psi(x)}{dx^2} + \left(\frac{2\pi\nu}{c}\mu\right)^2 \psi(x) = 0 \tag{6-52}$$

where the function $\psi(x)$ specifies the magnitude of the electric or magnetic field. When we compare this with the time-independent Schroedinger equation, written in the form

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi(x) = 0$$

we see that they are identical if the index of refraction in the former is connected with the potential energy function in the latter by the relation

$$\mu(x) = \frac{c}{2\pi\nu}\sqrt{\frac{2m}{\hbar^2}[E - V(x)]} \tag{6-53}$$

Thus the behavior of an optical system with index of refraction $\mu(x)$ should be identical to the behavior of a mechanical system with potential energy $V(x)$, providing the two functions are related as in (6-53). Indeed, there are optical phenomena which are exactly analogous to each of the quantum mechanical phenomena that arise in considering the motion of an unbound particle. An optical phenomenon, completely analogous to the total transmission of particles over barriers of length equal to an integral or half-integral number of wavelengths, is used in the coating of lenses to obtain very high light transmissions and in thin film optical filters.

An optical analogue to the penetration of barriers by particles is found in the imaginary indices of refraction that arise in total internal reflection. Consider a ray of light incident upon a glass-to-air interface at an angle greater than the critical angle θ_c. The resulting behavior of the light ray is called *total internal reflection*, and it is illustrated in the top of Figure 6-16. A detailed treatment of the process in terms of electromagnetic theory shows that the index of refraction, measured along the line ABC, is real in the region AB but imaginary in the region BC. Note that an imaginary $\mu(x)$ is suggested by (6-53) for a region analogous to one in which $E < V(x)$. Furthermore, electromagnetic theory shows that there are electromagnetic vibrations in the region BC of exactly the same form as the decreasing exponential standing wave of (6-29) for the region where $E < V(x)$. The flux of energy (the Poynting vector) is zero in this electromagnetic standing wave, just as the flux of probability is zero in the quantum mechanical standing wave, so the light ray is totally reflected. However, if a

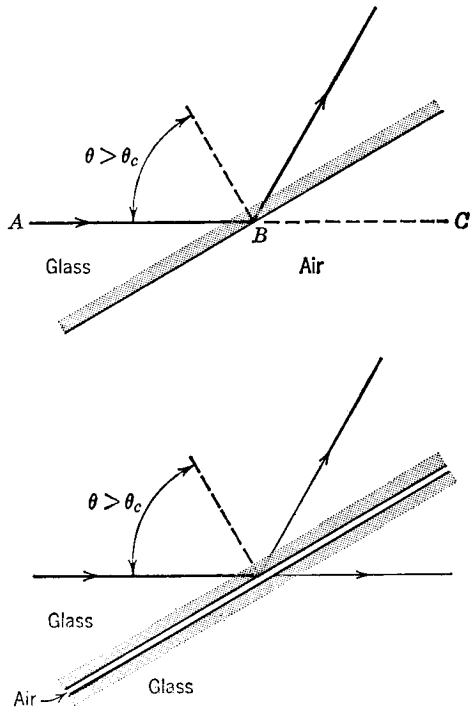


FIGURE 6-16

Top: Illustrating total internal reflection of a light ray. The angle of incidence is greater than the critical angle. *Bottom:* Illustrating frustrated total internal reflection. Some of the light ray is transmitted through the air gap if the gap is sufficiently narrow.

second block of glass is placed near enough to the first block to be in the region in which the electromagnetic vibrations are still appreciable, these vibrations are picked up and propagate through the second block. Furthermore, the electromagnetic vibrations in the air gap now carry a flux of energy through to the second block. This phenomenon, called *frustrated total internal reflection*, is illustrated in the bottom of Figure 6-16. Essentially the same thing happens in the quantum mechanical case when the region in which $E < V(x)$ is reduced from infinite thickness (step potential) to finite thickness (barrier potential). The transmission of light through an air gap, at an angle of incidence greater than the critical angle, was first observed by Newton around 1700. The equation relating the intensity of the transmitted beam to the thickness of the air gap, and other parameters, is identical in form to (6-49), and it has been verified experimentally.

It is particularly easy to observe frustrated total internal reflection of electromagnetic waves, using the microwave region of the spectrum and two blocks of paraffin separated by an air gap. Furthermore, careful inspection of the "ripple tank" photographs in Figures 6-17 and 6-18 will show that the phenomenon can even be observed with water waves. Frustrated total internal reflection, or its quantum mechanical equivalent barrier penetration, arises from properties common to all forms of classical or quantum mechanical wave motion.

6-6 Examples of Barrier Penetration by Particles

There are a number of interesting, and important, examples of barrier penetration by microscopic particles. A widespread, but not widely recognized, example is found in common household wiring. The usual way for an electrician to join two wires is to twist them together. Invariably there is a layer of copper oxide between the two wires, and this material is quite an effective insulator. Fortunately, the layer is extremely thin so the electrons flowing through the wire are able to tunnel through the layer by barrier penetration.

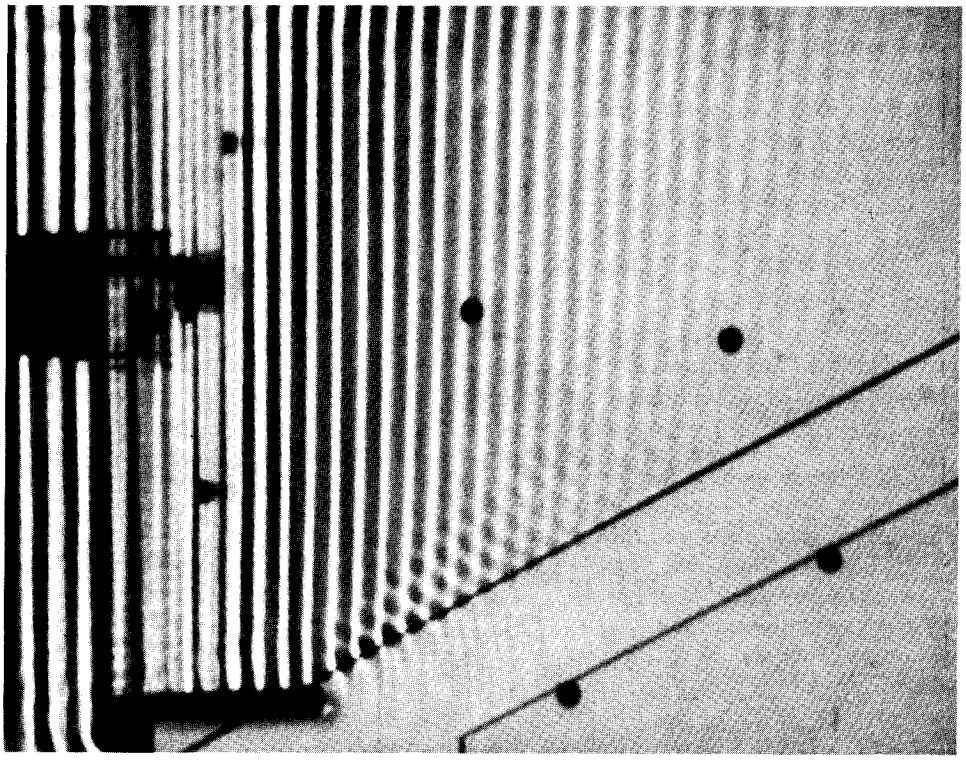


FIGURE 6-17

The total internal reflection of water waves. A long vibrating plunger on the left produces a set of waves in a region of shallow water, the waves being illuminated so as to make their crests easily visible. The waves are totally internally reflected at the diagonal boundary of a region where the layer of water abruptly becomes deeper, this reflection occurring because the velocity of water waves depends on the depth of the water. Note that the intensity of the waves decreases rapidly when they try to penetrate into the region of deeper water, but there is some penetration of that region. (Courtesy Film Studio, Education Development Center)

Historically, the first application of the quantum mechanical theory of barrier penetration by particles was to explain a long standing paradox concerning the emission of α particles in the decay of radioactive nuclei. As a typical example, consider the U^{238} nucleus. The potential energy $V(r)$ of an α particle at a distance r from the center of the nucleus had been investigated around 1910 by Rutherford, and others, who performed scattering experiments. Using as a probe the 8.8 MeV α particles emitted from the radioactive nuclei of Po^{212}, it was observed that their probability of scattering at various angles from U^{238} nuclei agreed with the predictions of Rutherford's scattering formula (see Chapter 4). The student will recall that that formula was based on the assumption that the interaction between the α particle and the nucleus strictly followed the Coulomb law repulsion that would be expected to operate between the two positively charged spherical objects. Thus Rutherford was able to conclude that, for the U^{238} nucleus, the potential function $V(r)$ felt by a neighboring α particle followed Coulomb's law, $V(r) = 2Ze^2/4\pi\epsilon_0 r$, where $2e$ is the α-particle charge and Ze is the nuclear charge—at least for distances greater than $r'' = 3 \times 10^{-14}$ m where $V(r'') = 8.8$ MeV, the probe α-particle energy. It was also known by scattering α particles from nuclei of light atoms that $V(r)$ eventually departs from a $1/r$ law when $r < r'$, the nuclear radius, although the exact value of r' was not known for the nuclei of heavy atoms at that time. Furthermore, since α

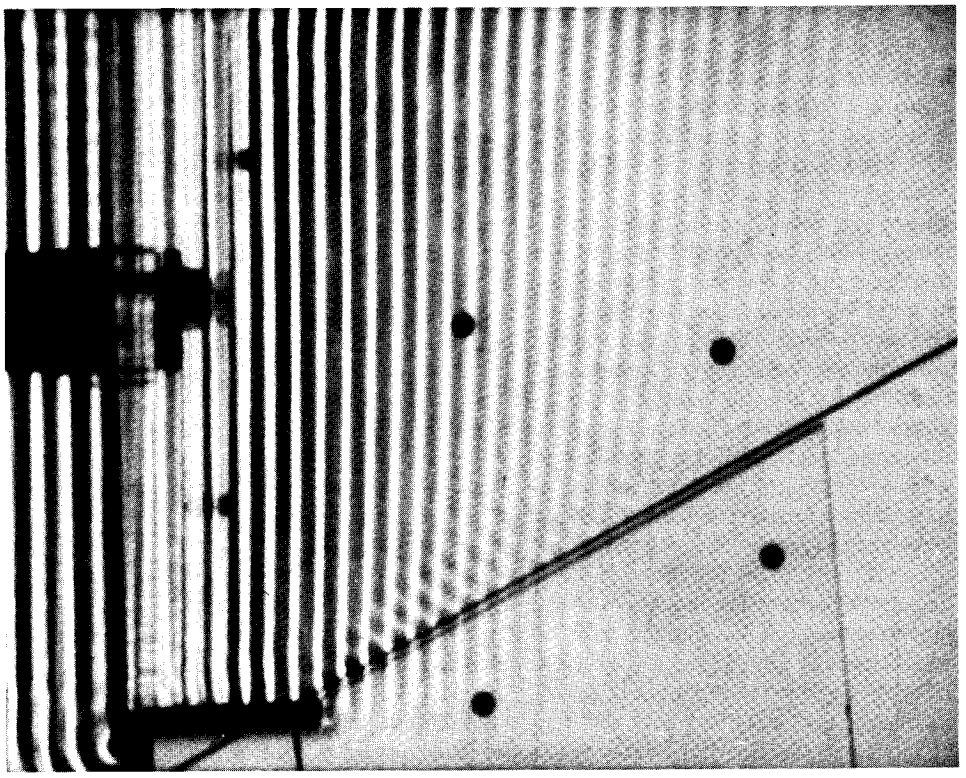


FIGURE 6-18

Frustrated total internal reflection of water waves. When the region of deeper water becomes a sufficiently narrow gap, the waves that have penetrated into the deeper water are picked up and transmitted into a second region of shallow water. (Courtesy Film Studio, Education Development Center)

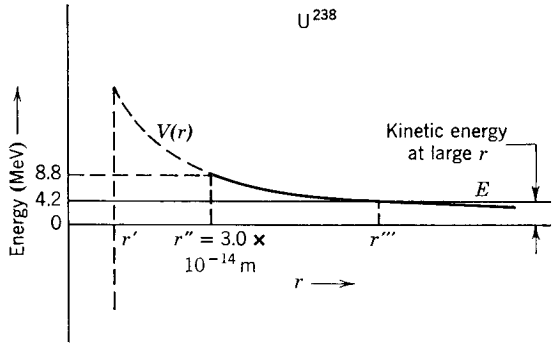
particles are occasionally emitted by U^{238} nuclei, it was assumed that they exist inside such nuclei, to which they are normally bound by the potential $V(r)$. From these arguments it was concluded that the form of $V(r)$ in the region $r < r''$ must be qualitatively as depicted in Figure 6-19. This conclusion has been verified by modern experiments involving the scattering of α particles produced by cyclotrons at energies high enough to allow the investigation of the potential over the entire range of r.

The paradox was connected with the fact that it was also known that the kinetic energy of α particles emitted in radioactive decay by U^{238} was 4.2 MeV. The kinetic energy was, of course, measured at a very large distance from the nucleus where $V(r) = 0$ and the kinetic energy equals the total energy E. This value of the constant total energy of the decay α particles emitted by U^{238} is also shown in Figure 6-19. From the point of view of classical mechanics, the situation was certainly paradoxical. An α particle of total energy E is initially in the region $r < r'$. This region is separated from the rest of space by a potential barrier of height which was known to be at least twice E. Yet it was observed that on occasion the α particle penetrates the barrier and moves off to large values of r.

To put it another way, according to classical mechanics an α particle emitted from a region where the potential energy function has the form shown in Figure 6-19 must, necessarily, have a much higher kinetic energy than was actually observed when it is far from the region. The reason is simply that in classical mechanics the total energy must be greater than the maximum value of the potential energy, if the particle is to escape the barrier. Consider the following analogy. You are walking beneath the span of a tall bridge, not looking up. Suddenly a brick

FIGURE 6-19

The potential energy V acting on an α particle at a distance r from the center of a U^{238} nucleus, and the total energy E of an α particle emitted from that radioactive nucleus. The solid part of the potential curve was known from scattering measurements to follow Coulomb's law into the distance of closest approach r'' of an 8.8 MeV α particle. The dashed part of the curve shows that the potential was assumed to continue to follow Coulomb's law into the nuclear radius r', where it must drop very rapidly to form a binding region. A 4.2 MeV α particle emitted from the radioactive nucleus must penetrate the potential barrier from the nuclear radius r' to the point at distance r''' from the center where its potential energy V becomes less than its total energy E.



hits you on the head, but gently, with a light tap. There is no place for the brick to come from, other than the bridge, but a brick falling from such a height would have developed enough kinetic energy to kill you!

In 1928 Gamow, Condon, and Gurney treated α particle emission as a quantum mechanical barrier penetration problem. They assumed that $V(r) = 2Ze^2/4\pi\epsilon_0 r$ for $r > r'$, where $2e$ is the α-particle charge and Ze is the charge of the nucleus remaining after the α particle is emitted. They also assumed that $V(r) < E$ for $r < r'$, as shown in Figure 6-19. Equation (6-50) was used to evaluate the transmission coefficient T since the exponent $k_{II}a$, which determines T, has a value large compared to one. In fact, the exponent is so large that the exponential completely dominates the behavior of T, and it was sufficient to take

$$T \simeq e^{-2k_{II}a} = e^{-2\sqrt{(2m/\hbar^2)(V_0-E)}\,a} \tag{6-54}$$

This expression was derived for a rectangular barrier of height V_0 and width a, but when the expression is valid it can be applied to the barrier $V(r)$ by considering it to be a set of adjacent rectangular barriers of height $V(r_i)$ and very small width Δr_i. This reasoning leads, in the limit, to the expression

$$T \simeq e^{-2\int_{r'}^{r'''}\sqrt{(2m/\hbar^2)[V(r)-E]}\,dr} \tag{6-55}$$

where the integration is taken from the nuclear radius r', where $V(r)$ rises above E, to the radius r''', where $V(r)$ drops below E. The use of (6-54), which was derived for a one-dimensional case, in (6-55) that concerns a three-dimensional problem, was justified because the α particles are almost always emitted with zero angular momentum. That is, they move out along essentially linear paths emanating from the nuclear center, obeying equations which are essentially one dimensional.

The quantity T gives the probability that in one trial an α particle will penetrate the barrier. The number of trials per second could be estimated to be

$$N \simeq \frac{v}{2r'} \tag{6-56}$$

if it were assumed that an α particle is bouncing back and forth with velocity v inside the nucleus of diameter $2r'$. Then the probability per second that the nucleus will decay by

emitting an α particle, called the decay rate R, would be

$$R \simeq \frac{v}{2r'} e^{-2\int_{r'}^{r'''} \sqrt{(2m/\hbar^2)(2Ze^2/4\pi\epsilon_0 r - E)}\, dr} \tag{6-57}$$

Today we know that (6-56) is not a very accurate estimate, but this function, or its more correct form, varies so slowly compared to the rapid variation in the exponential that the result expressed by (6-57) is an accurate estimate.

In applying (6-57) to a particular radioactive nucleus, Gamow, Condon, and Gurney took all the quantities in the expression as known, except v and r' (r''' can be evaluated from Z and E). Assuming v to be comparable to the velocity of the α particle after emission (i.e., $mv^2/2 = E$), the decay rate R is then a function only of the nuclear radius r'. Using $r' = 9 \times 10^{-15}$ m, which was certainly in line with the values obtained from Rutherford's analysis of α-particle scattering from light nuclei, they obtained values of R which were in good agreement with those measured experimentally, although the decay rate varies over a *tremendously* large range. As an example, for U^{238}, the decay rate is $R = 5 \times 10^{-18}$ sec^{-1}. An example at the other extreme is Po^{212}, for which $R = 2 \times 10^{6}$ sec^{-1}. This variation in R is due primarily to the variation, from one radioactive nucleus to the next, of the energy E of the emitted α particles. The height of the barrier and the nuclear radius do not change significantly for nuclei in the limited range of the periodic table in which α-emitting nuclei are found. A comparison between experiment and theory is shown in Figure 6-20. The successful application of Schroedinger quantum mechanics to the α-particle emission paradox provided one of its earliest, and most convincing, verifications.

Barrier penetration of atoms takes place in the periodic *inversion* of the ammonia molecule, NH_3. Figure 6-21 illustrates schematically the structure of this molecule. It consists of three H atoms arranged in a plane, and equidistant from the N atom. There are two completely equivalent equilibrium positions for the N atom, one on either side of the plane containing the H atoms. Figure 6-22 indicates the potential energy acting on the N atom, as a function of its distance x from that plane. The potential function $V(x)$ has two minima, corresponding to the two equilibrium positions, which are symmetrically disposed about a low maximum located at $x = 0$. This maximum, which constitutes a barrier separating the two binding regions, arises from the repulsive Coulomb forces that act on the N atom if it penetrates the plane of the H atoms. The forces are strong enough that in classical mechanics the N atom is not able to cross the barrier, if the molecule is in one of its low-lying energy states; that is, the

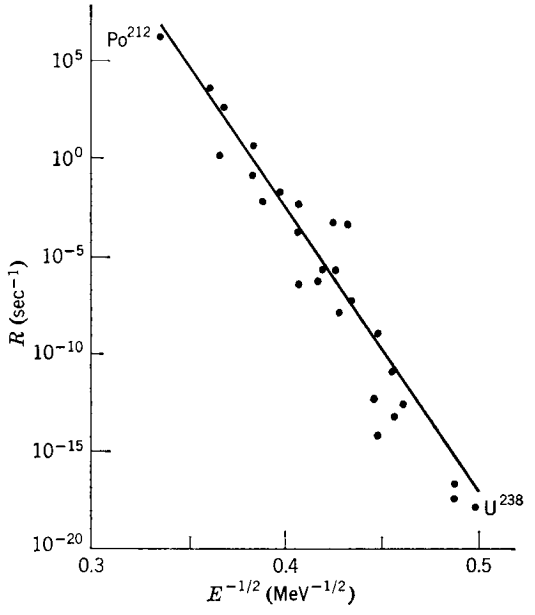


FIGURE 6-20

The probability per second R that a radioactive nucleus will emit an α particle of energy E. The points are experimental measurements and the solid curve is the prediction of (6-57), a result of barrier penetration theory.

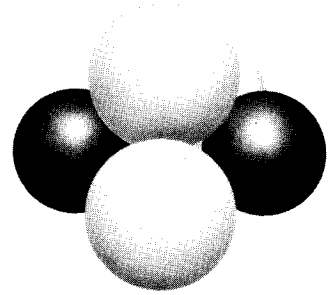


FIGURE 6-21
A schematic illustration of the NH_3 molecule. The light spheres represent the three H atoms arranged in a plane. The dark spheres represent two equivalent equilibrium positions of the single N atom.

lower allowed energies of this binding potential are below the top of the barrier, as indicated in the figure. But penetration of the classically excluded region allows the N atom to tunnel through the barrier. If it is initially on one side, it will tunnel through and eventually appear on the other side. Then it will do it again in the opposite direction. The N atom actually oscillates slowly back and forth across the plane of the H atoms. The oscillation frequency is $\nu = 2.3786 \times 10^{10}$ Hz, when the molecule is in its ground state. This frequency is much lower than those found in molecular vibrations not involving barrier penetration, or in other atomic or molecular phenomena. Due to the resulting technical simplifications, the frequency was used as a standard in the first atomic clocks which measure time with maximum precision.

A recent, and very useful, example of barrier penetration of electrons is found in the *tunnel diode*. This is a semiconductor device, like a transistor, which is used in fast electronic circuits since its high frequency response is much better than that of any transistor. The operation of a tunnel diode will be explained in Chapter 13, in the context of a discussion of semiconductors. So here we shall say only that the device employs controllable barrier penetration to switch currents on or off so rapidly that it can be used to make an oscillator that can operate at frequencies above 10^{11} Hz.

6-7 The Square Well Potential

In the preceding sections we have treated the motion of particles in potentials which are not capable of binding them to limited regions of space. Although a number of

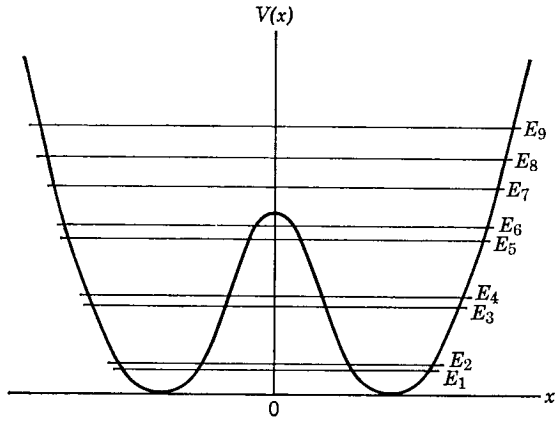


FIGURE 6-22
The potential energy of the N atom in the NH_3 molecule, as a function of its distance from the plane containing the three H atoms, which lies at $x = 0$. In its lower energy states, the total energy of the molecule lies below the top of the barrier separating the two minima, as indicated by the eigenvalues of the potential shown in the figure.