7 Tunneling Phenomena

Chapter Outline

In this chapter the principles of wave mechanics are applied to particles striking a potential *barrier*. Unlike potential wells that attract and trap particles, barriers repel them. Because barriers have no bound states, the emphasis shifts to determining whether a particle incident on a barrier is reflected or transmitted.

In the course of this study we shall encounter a peculiar phenomenon called *tunneling*. A purely wave-mechanical effect, tunneling nevertheless is essential to the operation of many modern-day devices and shapes our world on a scale from atomic all the way up to galactic proportions. The chapter includes a discussion of the role played by tunneling in several phenomena of practical interest, such as field emission, radioactive decay, and the operation of the ammonia maser. Finally, the chapter is followed by an essay on the scanning tunneling microscope, or STM, a remarkable device that uses tunneling to make images of surfaces with resolution comparable to the size of a single atom.

7.1 THE SQUARE BARRIER

The square barrier is represented by a potential energy function $U(x)$ that is constant at U in the barrier region, say between $x = 0$ and $x = L$, and zero outside this region. One method for producing a square barrier potential using charged hollow cylinders is shown in Figure 7.1a. The outer cylinders are grounded while the central one is held at some positive potential V. For a particle with charge q, the barrier potential energy is $U = qV$. The

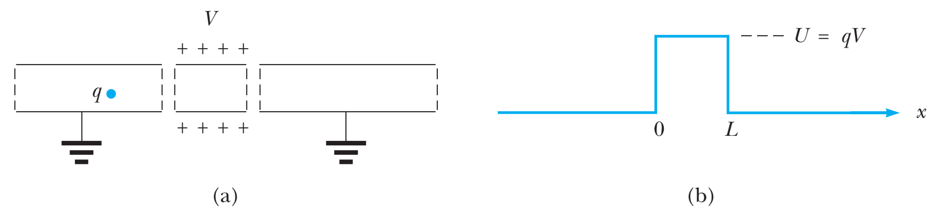

Figure 7.1 (a) Aligned metallic cylinders serve as a potential barrier to charged particles. The central cylinder is held at some positive electric potential V, and the outer cylinders are grounded. A charge q whose total energy is less than qV is unable to penetrate the central cylinder classically, but can do so quantum mechanically by a process called tunneling. (b) The potential energy seen by this charge in the limit where the gaps between the cylinders have shrunk to zero size. The result is the square barrier potential of height U.

charge experiences no electric force except in the gaps separating the cylinders. The force in the gaps is repulsive, tending to expel a positive charge q from the central cylinder. The electric potential energy for the idealized case in which the gaps have shrunk to zero size is the **square barrier,** sketched in Figure 7.1b.

A classical particle incident on the barrier, say from the left, experiences a retarding force on arriving at $x = 0$. Particles with energies E greater than U are able to overcome this force, but suffer a reduction in speed to a value commensurate with their diminished kinetic energy $(E - U)$ in the barrier region. Such particles continue moving to the right with reduced speed until they reach $x = L$, where they receive a "kick" accelerating them back to their original speed. Thus, particles having energy $E > U$ are able to cross the barrier with their speed restored to its initial value. By contrast, particles with energy $E < U$ are turned back (reflected) by the barrier, having insufficient energy to cross or even penetrate it. In this way the barrier divides the space into classically allowed and forbidden regions determined by the particle energy: If $E > U$, the whole space is accessible to the particle; for $E < U$ only the interval to the side of the barrier in which the particle originates is accessible—the barrier region itself is forbidden, and this precludes particle motion on the far side as well.

According to quantum mechanics, however, **there is no region inaccessible to our particle, regardless of its energy,** since the matter wave associated with the particle is nonzero everywhere. A typical wavefunction for this case, illustrated in Figure 7.2a, clearly shows the penetration of the wave into the barrier and beyond. This barrier penetration is in complete disagreement with classical physics. The process of penetrating the barrier is called **tunneling:** we say the particle has tunneled through the barrier.

The mathematical expression for Ψ on either side of the barrier is easily found. To the left of the barrier the particle is free, so the wavefunction here is composed of the free particle plane waves introduced in Chapter 6:

$$\Psi(x, t) = Ae^{i(kx - \omega t)} + Be^{i(-kx - \omega t)} \tag{7.1}$$

This wavefunction $\Psi(x, t)$ is actually the sum of two plane waves. Both have frequency ω and energy $E = \hbar\omega = \hbar^2 k^2/2m$, but the first moves from left to right (wavenumber k), the second from right to left (wavenumber $-k$). Thus,

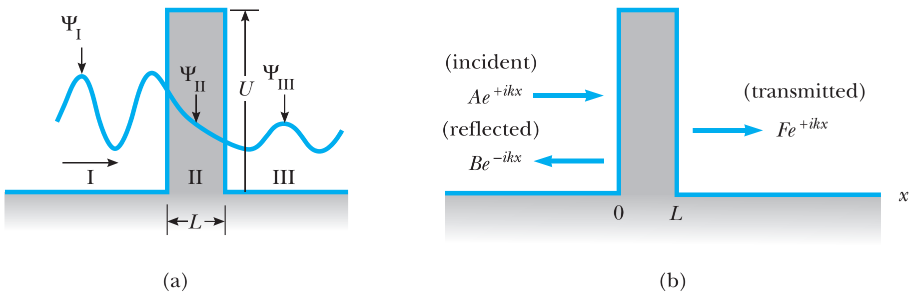

Figure 7.2 (a) A typical stationary-state wave for a particle in the presence of a square barrier. The energy E of the particle is less than the barrier height U. Since the wave amplitude is nonzero in the barrier, there is some probability of finding the particle there. (b) Decomposition of the stationary wave into incident, reflected, and transmitted waves.

that part of Ψ proportional to A is interpreted as a wave incident on the barrier from the left; that proportional to B as a wave reflected from the barrier and moving from right to left (Fig. 7.2b). The **reflection coefficient** R for the barrier is calculated as the ratio of the reflected probability density to the incident probability density:

$$R = \frac{(\Psi^*\Psi)_{\text{reflected}}}{(\Psi^*\Psi)_{\text{incident}}} = \frac{B^*B}{A^*A} = \frac{|B|^2}{|A|^2} \tag{7.2}$$

Reflection coefficient for a barrier

In wave terminology, R is the fraction of wave intensity in the reflected beam; in particle language, R becomes the likelihood (probability) that a particle incident on the barrier from the left is reflected by it.

Similar arguments apply to the right of the barrier, where, again, the particle is free:

$$\Psi(x, t) = Fe^{i(kx-\omega t)} + Ge^{i(-kx-\omega t)} \tag{7.3}$$

This form for $\Psi(x, t)$ is valid in the range $x > L$, with the term proportional to F describing a wave traveling to the right, and that proportional to G a wave traveling to the left in this region. The latter has no physical interpretation for waves incident on the barrier from the left, and so is discarded by requiring $G = 0$. The former is that part of the incident wave that is transmitted through the barrier. The relative intensity of this transmitted wave is the **transmission coefficient** for the barrier T:

$$T = \frac{(\Psi^*\Psi)_{\text{transmitted}}}{(\Psi^*\Psi)_{\text{incident}}} = \frac{F^*F}{A^*A} = \frac{|F|^2}{|A|^2} \tag{7.4}$$

Transmission coefficient for a barrier

The transmission coefficient measures the likelihood (probability) that a particle incident on the barrier from the left penetrates to emerge on the other side. Since a particle incident on the barrier is either reflected or transmitted, the probabilities for these events must sum to unity:

$$R + T = 1 \tag{7.5}$$

Equation 7.5 expresses a kind of **sum rule** obeyed by the barrier coefficients. Further, the degree of transmission or reflection will depend on particle energy. In the classical case $T = 0$ (and $R = 1$) for $E < U$, but $T = 1$ (and $R = 0$) for $E > U$. The wave-mechanical predictions for the functions $T(E)$ and $R(E)$ are more complicated; to obtain them we must examine the matter wave within the barrier.

To find Ψ in the barrier, we must solve Schrödinger's equation. Let us consider stationary states $\psi(x)e^{-i\omega t}$ whose energy $E = \hbar\omega$ is below the top of the barrier. This is the case $E < U$ for which no barrier penetration is permitted classically. In the region of the barrier ($0 < x < L$), $U(x) = U$ and the time-independent Schrödinger equation for $\psi(x)$ can be rearranged as

$$\frac{d^2\psi}{dx^2} = \left\{\frac{2m(U-E)}{\hbar^2}\right\}\psi(x)$$

With $E < U$, the term in braces is a positive constant, and solutions to this equation are the *real exponential* forms $e^{\pm\alpha x}$. Since $(d^2/dx^2)e^{\pm\alpha x} = (\alpha)^2 e^{\pm\alpha x}$, we should identify the term in braces with α^2 or, equivalently,

$$\alpha = \frac{\sqrt{2m(U-E)}}{\hbar} \tag{7.6}$$

For wide barriers, the probability of finding the particle should decrease steadily into the barrier; in such cases only the decaying exponential is important, and it is convenient to define a barrier **penetration depth** $\delta = 1/\alpha$. At a distance δ into the barrier, the wavefunction has fallen to $1/e$ of its value at the barrier edge; thus, the probability of finding the particle is appreciable only within about δ of the barrier edge.

The complete wavefunction in the barrier is, then,

$$\Psi(x, t) = \psi(x)e^{-i\omega t} = Ce^{-\alpha x - i\omega t} + De^{+\alpha x - i\omega t} \qquad \text{for } 0 < x < L \tag{7.7}$$

The coefficients C and D are fixed by requiring smooth joining of the wavefunction across the barrier edges; that is, both Ψ and $\partial\Psi/\partial x$ must be continuous at $x = 0$ and $x = L$. Writing out the joining conditions using Equations 7.1, 7.3, and 7.7 for Ψ in the regions to the left, to the right, and within the barrier, respectively, gives

Joining conditions at a square barrier

$$\begin{aligned}
A + B &= C + D && \text{(continuity of } \Psi \text{ at } x = 0) \\
ikA - ikB &= \alpha D - \alpha C && \left(\text{continuity of } \frac{\partial\Psi}{\partial x} \text{ at } x = 0\right) \\
Ce^{-\alpha L} + De^{+\alpha L} &= Fe^{ikL} && \text{(continuity of } \Psi \text{ at } x = L) \\
(\alpha D)e^{+\alpha L} - (\alpha C)e^{-\alpha L} &= ikFe^{ikL} && \left(\text{continuity of } \frac{\partial\Psi}{\partial x} \text{ at } x = L\right)
\end{aligned} \tag{7.8}$$

In keeping with our previous remarks, we have set $G = 0$. Still, there is one more unknown than there are equations to find them. Actually this is as it should be, since the amplitude of the incident wave merely sets the scale for the other amplitudes. That is, doubling the incident wave amplitude simply doubles the amplitudes of the reflected and transmitted waves. Dividing Equations 7.8 through by A furnishes four equations for the four ratios B/A, C/A, D/A, and F/A. These equations may be solved by repeated substitution to find B/A and so on in terms of the barrier height U, the barrier width L, and the particle energy E. The result for the transmission coefficient T is (see Problem 7)

$$T(E) = \left\{1 + \frac{1}{4}\left[\frac{U^2}{E(U-E)}\right]\sinh^2 \alpha L\right\}^{-1} \tag{7.9}$$

where sinh denotes the hyperbolic sine function: $\sinh x = (e^x - e^{-x})/2$.

A sketch of $T(E)$ for the square barrier is shown in Figure 7.3. Equation 7.9 holds only for energies E below the barrier height U. For $E > U$, α becomes imaginary and $\sinh(\alpha L)$ turns oscillatory. This leads to fluctuations in $T(E)$ and isolated energies for which transmission occurs with complete certainty, that is, $T(E) = 1$. Such *transmission resonances* arise from wave interference and constitute further evidence for the wave nature of matter (see Example 7.3).

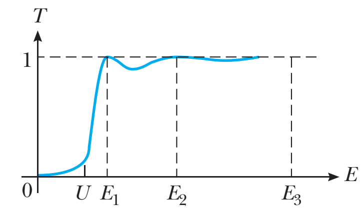

Figure 7.3 A sketch of the transmission coefficient $T(E)$ for a square barrier. Oscillation in $T(E)$ with E, and the transmission resonances at E_1, E_2, and E_3, are further evidence for the wave nature of matter.

EXAMPLE 7.1 Transmission Coefficient for an Oxide Layer

Two copper conducting wires are separated by an insulating oxide layer (CuO). Modeling the oxide layer as a square barrier of height 10.0 eV, estimate the transmission coefficient for penetration by 7.00-eV electrons (a) if the layer thickness is 5.00 nm and (b) if the layer thickness is 1.00 nm.

Solution From Equation 7.6 we calculate α for this case, using $\hbar = 1.973 \text{ keV}\cdot\text{Å}/c$ and $m_e = 511 \text{ keV}/c^2$ for electrons to get

$$\alpha = \frac{\sqrt{2m_e(U-E)}}{\hbar}$$

$$= \frac{\sqrt{2(511 \text{ keV}/c^2)(3.00 \times 10^{-3} \text{ keV})}}{1.973 \text{ keV}\cdot\text{Å}/c} = 0.8875 \text{ Å}^{-1}$$

The transmission coefficient from Equation 7.9 is then

$$T = \left\{1 + \frac{1}{4}\left[\frac{10^2}{7(3)}\right]\sinh^2(0.8875 \text{ Å}^{-1})L\right\}^{-1}$$

Substituting $L = 50.0$ Å (5.00 nm) gives

$$T = 0.963 \times 10^{-38}$$

a fantastically small number on the order of 10^{-38}! With $L = 10.0$ Å (1.00 nm), however, we find

$$T = 0.657 \times 10^{-7}$$

We see that reducing the layer thickness by a factor of 5 enhances the likelihood of penetration by nearly 31 orders of magnitude!

Exercise 1 Go to our companion Web site (http://info.brookscole.com/mp3e) and select QMTools Simulations → Exercise 7.1. This particular Java applet shows the de Broglie wave (actually, just the real part) for an electron with energy 7.00 eV incident from the left on a square barrier 10.0 eV high and 1.0 Å wide. Compare this waveform with the illustration of Figure 7.2a. In fact, this wave is inherently complex valued, with a modulus and phase that varies from point to point. A more informative display plots the modulus in the usual way but uses color to represent the phase of the wave. Right-click on the waveform and select Properties . . . → Color-4-Phase → Apply to show the color-for-phase plotting style. Why does the transmitted wave (to the right of the barrier) now have a uniform height? What is the significance of this height? Follow the on-site instructions to display the incident component of this scattering wave and determine the transmission coefficient directly from the graphs. Compare your result with the prediction of Equation 7.9.

EXAMPLE 7.2 Tunneling Current Through an Oxide Layer

A 1.00-mA current of electrons in one of the wires of Example 7.1 is incident on the oxide layer. How much of this current passes through the layer to the adjacent wire if the electron energy is 7.00 eV and the layer thickness is 1.00 nm? What becomes of the remaining current?

Solution Because each electron carries a charge equal to $e = 1.60 \times 10^{-19}$ C, an electron current of 1.00 mA represents $10^{-3}/(1.60 \times 10^{-19}) = 6.25 \times 10^{15}$ electrons per second impinging on the barrier. Of these, only the fraction T is transmitted, where $T = 0.657 \times 10^{-7}$ from Example 7.1. Thus, the number of electrons per second continuing on to the adjacent wire is

$$(6.25 \times 10^{15})(0.657 \times 10^{-7}) = 4.11 \times 10^{8} \text{ electrons/s}$$

This number represents a transmitted current of

$$\begin{aligned}(4.11 \times 10^{8}/\text{s})(1.60 \times 10^{-19}\text{ C}) &= 6.57 \times 10^{-11}\text{ A} \\ &= 65.7\text{ pA (picoamperes)}\end{aligned}$$

(Notice that the same transmitted current would be obtained had we simply multiplied the incident current by the transmission coefficient.) The remaining 1.00 mA − 65.7 pA is reflected at the layer. It is important to note that the *measured* conduction current in the wire on the side of incidence is the net of the incident and reflected currents, or again 65.7 pA.

EXAMPLE 7.3 Transmission Resonances

Consider a particle incident from the left on a square barrier of width L in the case where the particle energy E exceeds the barrier height U. Write the necessary wavefunctions and impose the proper joining conditions to obtain a formula for the transmission coefficient for this case. Show that perfect transmission (resonance) results for special values of particle energy, and explain this phenomenon in terms of the interference of de Broglie waves.

Solution To the left and right of the barrier, the wavefunctions are the free particle waves given by Equations 7.1 and 7.3 (again with $G = 0$ to describe a purely transmitted wave on the far side of the barrier):

$$\Psi(x, t) = Ae^{i(kx-\omega t)} + Be^{i(-kx-\omega t)} \qquad x < 0$$

$$\Psi(x, t) = Fe^{i(kx-\omega t)} \qquad x > L$$

The wavenumber k and frequency ω of these oscillations derive from the particle energy E in the manner characteristic of (nonrelativistic) de Broglie waves; that is, $E = (\hbar k)^2/2m = \hbar\omega$. Within the barrier, the wavefunction also is oscillatory. In effect, the decay constant α of Equation 7.6 has become imaginary, since $E > U$. Introducing a new wavenumber k' as $\alpha = ik'$, the barrier wavefunction becomes

$$\Psi(x, t) = Ce^{i(-k'x-\omega t)} + De^{i(k'x-\omega t)} \qquad 0 < x < L$$

with $k' = [2m(E-U)/\hbar^2]^{1/2}$ a real number.

The barrier wavefunction will join smoothly to the exterior waveforms if the wavefunction and its slope are continuous at the barrier edges $x = 0$ and $x = L$. These continuity requirements are identical to Equations 7.8 with the replacement $\alpha = ik'$ everywhere. In particular, we now have

$$A + B = C + D \qquad (\text{continuity of } \Psi \text{ at } x = 0)$$

$$kA - kB = k'D - k'C \qquad \left(\text{continuity of } \frac{\partial\Psi}{\partial x} \text{ at } x = 0\right)$$

$$Ce^{-ik'L} + De^{ik'L} = Fe^{ikL} \qquad (\text{continuity of } \Psi \text{ at } x = L)$$

$$k'De^{ik'L} - k'Ce^{-ik'L} = kFe^{ikL} \qquad \left(\text{continuity of } \frac{\partial\Psi}{\partial x} \text{ at } x = L\right)$$

To isolate the transmission amplitude F/A, we must eliminate from these relations the unwanted coefficients B, C, and D. Dividing the second line by k and adding to the first eliminates B, leaving A in terms of C and D. In the same way, dividing the fourth line by k' and adding the result to the third line gives D (in terms of F), while subtracting the result from the third line gives C (in terms of F). Combining the previous results finally yields A in terms of F:

$$A = \frac{1}{4}Fe^{ikL}\left\{\left[2 - \left(\frac{k'}{k} + \frac{k}{k'}\right)\right]e^{ik'L} + \left[2 + \left(\frac{k'}{k} + \frac{k}{k'}\right)\right]e^{-ik'L}\right\}$$

The transmission probability is $T = |F/A|^2$. Writing $e^{\pm ik'L} = \cos k'L \pm i \sin k'L$ and simplifying, we obtain the final result

$$\begin{aligned}\frac{1}{T} = \left|\frac{A}{F}\right|^2 &= \frac{1}{4}\left|2\cos k'L - i\left(\frac{k'}{k} + \frac{k}{k'}\right)\sin k'L\right|^2 \\ &= 1 + \frac{1}{4}\left[\frac{U^2}{E(E-U)}\right]\sin^2 k'L\end{aligned}$$

We see that **transmission resonances** occur whenever $k'L$ is a multiple of π. Using $k' = [2m(E-U)/\hbar^2]^{1/2}$, we can express the resonance condition in terms of the particle energy E as

$$E = U + n^2\frac{\pi^2\hbar^2}{2mL^2} \qquad n = 1, 2, \ldots$$

Particles with these energies are transmitted perfectly ($T = 1$), with no chance of reflection ($R = 0$).

Resonances arise from the interference of the matter wave accompanying a particle. The wave reflected from the barrier can be regarded as the superposition of matter waves reflected from the leading and trailing edges of the barrier at $x = 0$ and $x = L$, respectively. If these reflected waves arrive phase shifted by odd multiples of 180° or π radians, they will interfere destructively, leaving no reflected wave ($R = 0$) and thus perfect transmission. Now the wave reflected from the rear of the barrier at $x = L$ must travel the extra distance $2L$ before recombining with the wave reflected at the front, leading to a phase difference of $2k'L$. But this wave also suffers an intrinsic phase shift of π radians, having been reflected from a medium with higher optical density.[1] Thus, the condition for destructive interference becomes $2k'L + \pi = (2n + 1)\pi$, or simply $k'L = n\pi$, where $n = 1, 2, \ldots$.

Perfect transmission also arises when particles are scattered by a potential well, a phenomenon known as the **Ramsauer–Townsend effect** (see Problem 11).

Exercise 2 Verify that for $E >> U$, the transmission coefficient of Example 7.3 approaches unity. Why is this result expected? What happens to T in the limit as E approaches U?

EXAMPLE 7.4 Scattering by a Potential Step

The potential step shown in Figure 7.4 may be regarded as a square barrier in the special case where the barrier width L is infinite. Apply the ideas of this section to discuss the quantum scattering of particles incident from the left on a potential step, in the case where the step height U exceeds the total particle energy E.

Solution The wavefunction everywhere to the right of the origin is the barrier wavefunction given by Equation 7.7. To keep Ψ from diverging for large x, we must take $D = 0$, leaving only the decaying wave

$$\Psi(x, t) = Ce^{-\alpha x - i\omega t} \qquad x > 0$$

This must be joined smoothly to the wavefunction on the left of the origin, given by Equation 7.1:

$$\Psi(x, t) = Ae^{ikx - i\omega t} + Be^{-ikx - i\omega t} \qquad x < 0$$

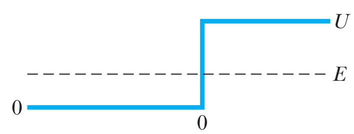

Figure 7.4 (Example 7.4) The potential step of height U may be thought of as a square barrier of the same height in the limit where the barrier width L becomes infinite. All particles incident on the barrier with energy $E < U$ are reflected.

The conditions for smooth joining at $x = 0$ yield

$$A + B = C \qquad \text{(continuity of } \Psi)$$

$$ikA - ikB = -\alpha C \qquad \left(\text{continuity of } \frac{\partial \Psi}{\partial x}\right)$$

Solving the second equation for C and substituting into the first (with $\delta = 1/\alpha$) gives $A + B = -ik\delta A + ik\delta B$, or

$$\frac{B}{A} = -\frac{(1 + ik\delta)}{(1 - ik\delta)}$$

The reflection coefficient is $R = |B/A|^2 = (B/A)(B/A)^*$, or

$$R = \left(\frac{(1 + ik\delta)}{(1 - ik\delta)}\right)\left(\frac{(1 - ik\delta)}{(1 + ik\delta)}\right) = 1$$

Thus, an *infinitely* wide barrier reflects all incoming particles with energies below the barrier height, in agreement with the classical prediction. Nevertheless, there is a nonzero wave in the step region since

$$\frac{C}{A} = 1 + \frac{B}{A} = \frac{-2ik\delta}{1 - ik\delta} \neq 0$$

But the wavefunction for $x > 0$, $\Psi(x, t) = Ce^{-\alpha x - i\omega t}$, is not a propagating wave at all; that is, there is no net transmission of particles to the right of the step. However, there will be quantum transmission through a barrier of *finite* width, no matter how wide (compare Eq. 7.9).

[1]This is familiar from the propagation of classical waves: A traveling wave arriving at the interface separating two media is partially transmitted and partially reflected. The reflected portion is phase shifted 180° only in the case where the wave speed is lower in the medium being penetrated. For matter waves, $p = h/\lambda$, and the wavelength (hence, wave speed) is largest in regions where the kinetic energy is smallest. Thus, the matter wave reflected from the front of a barrier suffers no change in phase, but that reflected from the rear is phase shifted 180°.

Figure 7.5 (a) Total internal reflection of light waves at a glass–air boundary. An evanescent wave penetrates into the space beyond the reflecting surface. (b) Frustrated total internal reflection. The evanescent wave is "picked up" by a neighboring surface, resulting in transmission across the gap. Notice that the light beam *does not* appear in the gap.

The existence of a barrier wave without propagation (as in Example 7.4) is familiar from the optical phenomenon of total internal reflection exploited in the construction of beam splitters (Figure 7.5): Light entering a right-angle prism is completely reflected at the hypotenuse face, even though an electromagnetic wave, the evanescent wave, penetrates into the space beyond. A second prism brought into near contact with the first can "pick up" this evanescent wave, thereby transmitting and redirecting the original beam (Fig. 7.5b). This phenomenon, known as **frustrated total internal reflection,** is the optical analog of tunneling: In effect, photons have tunneled across the gap separating the two prisms.

7.2 BARRIER PENETRATION: SOME APPLICATIONS

In actuality, few barriers can be modeled accurately using the square barrier discussed in the preceding section. Indeed, the extreme sensitivity to barrier constants found there suggests that barrier shape will be important in making reliable predictions of tunneling probabilities. The transmission coefficient for a barrier of arbitrary shape, as specified by some potential energy function $U(x)$, can be found from Schrödinger's equation. For high, wide barriers, where the likelihood of penetration is small, a lengthy treatment yields the approximate result

Approximate transmission coefficient of a barrier with arbitrary shape

$$T(E) \approx \exp\left(-\frac{2}{\hbar}\sqrt{2m}\int\sqrt{U(x)-E}\,dx\right) \tag{7.10}$$

The integral in Equation 7.10 is taken over the classically forbidden region where $E < U(x)$. A simple argument leading to this form follows by representing an arbitrary barrier as a succession of square barriers, all of which scatter independently, so that the transmitted wave intensity of one becomes the incident wave intensity for the next, and so forth (see Problem 15).

The use of Equation 7.10 is illustrated in the remainder of this section, where it is applied to several classic problems in contemporary physics.

Field Emission

In field emission, electrons bound to a metal are literally torn from the surface by the application of a strong electric field. In this way, the metal becomes a source that may be conveniently tapped to furnish electrons for many applications. In the past, such cold cathode emission, as it was known, was a popular way of generating electrons in vacuum tube circuits, producing less electrical "noise" than hot filament sources, where electrons were "boiled off" by heating the metal to a high temperature. Modern applications include the **field emission microscope** (Fig. 7.6) and a related device, the **scanning tunneling microscope** (see the essay at the end of this chapter), both of which use the escaping electrons to form an image of structural details at the emitting surface.

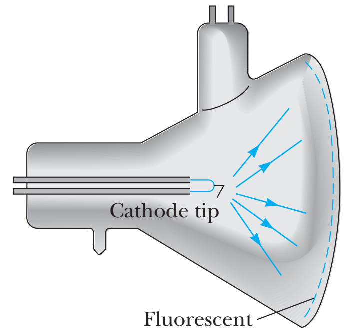

Figure 7.6 Schematic diagram of a field emission microscope. The intense electric field at the tip of the needle-shaped specimen allows electrons to tunnel through the work function barrier at the surface. Since the tunneling probability is sensitive to the exact details of the surface where the electron passes, the number of escaping electrons varies from point to point with the surface condition, thus providing a picture of the surface under study.

Field emission is a tunneling phenomenon. Figure 7.7a shows schematically how field emission can be obtained by placing a positively charged plate near the source metal to form, effectively, a parallel-plate capacitor. In the gap between the "plates" there is some electric field $\mathcal{E}$, but the electric field inside the metal remains zero due to the shielding by the mobile metal electrons attracted to the surface by the positively charged plate. Note that an electron in the bulk is virtually free, yet still bound to the metal by a potential well of depth U. The total electron energy E, which includes kinetic energy, is negative to indicate a bound electron; indeed, $|E|$ represents the energy needed to free this electron, a value at least equal to the work function of the metal.

Tunneling model for field emission

Once beyond the surface ($x > 0$), our electron is attracted by the electric force in the gap, $F = e\mathcal{E}$, represented by the potential energy $U(x) = -e\mathcal{E}x$. The potential energy diagram is shown in Figure 7.7b, together with the classically allowed and forbidden regions for an electron of energy E. The intersections of E with $U(x)$ at x_1 ($= 0$) and x_2 ($= -E/e\mathcal{E}$) mark the classical turning points, where a classical particle with this energy would be turned around to keep it from entering the forbidden zone. Thus, from a classical viewpoint, an electron initially confined to the metal has insufficient energy to surmount the potential barrier at the surface and would remain in the bulk forever! It is only by virtue of its wave character that the electron can tunnel through this barrier to emerge on the other side. The probability of such an occurrence is measured by the transmission coefficient for the triangular barrier depicted in Figure 7.7b.

To calculate $T(E)$ we must evaluate the integral in Equation 7.10 over the classically forbidden region from x_1 to x_2. Since $U(x) = -e\mathcal{E}x$ in this region and $E = -e\mathcal{E}x_2$, we have

$$\int \sqrt{U(x) - E}\, dx = \sqrt{e\mathcal{E}} \int_0^{x_2} \sqrt{x_2 - x}\, dx$$

$$= -\frac{2}{3}\sqrt{e\mathcal{E}}\,\{x_2 - x\}^{3/2}\Big|_0^{x_2} = \frac{2}{3}\sqrt{e\mathcal{E}}\left(\frac{|E|}{e\mathcal{E}}\right)^{3/2}$$

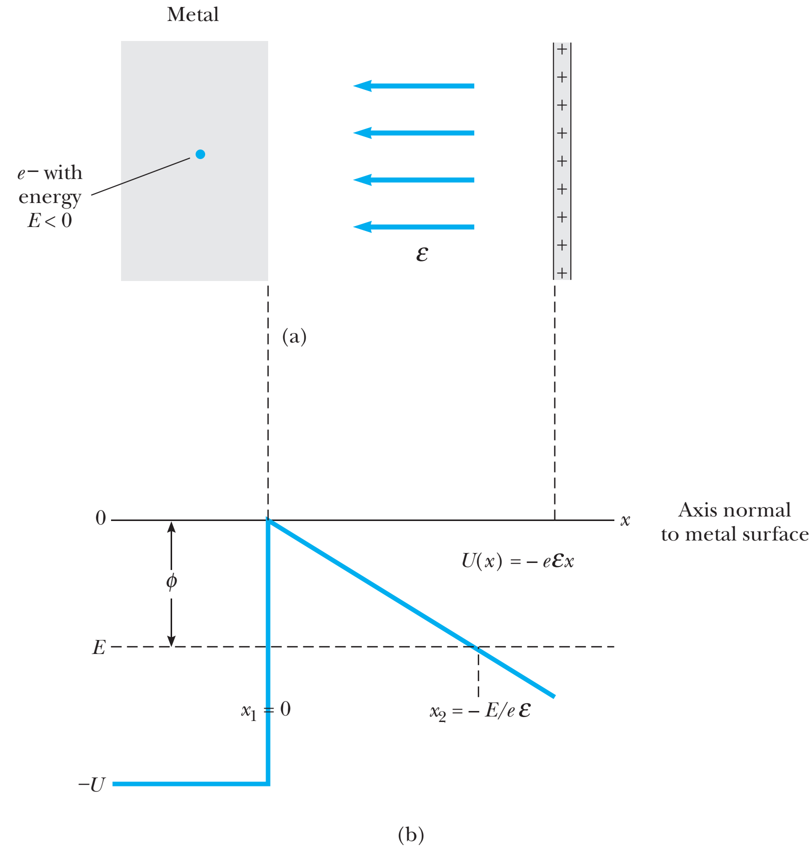

Figure 7.7 (a) Field emission from a metal surface. (b) The potential energy seen by an electron of the metal. The electric field produces the triangular potential barrier shown, through which electrons can tunnel to escape the metal. Turning points at $x_1 = 0$ and $x_2 = -E/e\mathcal{E}$ delineate the classically forbidden region. (Note that x_2 is positive since E is negative.) Tunneling is greatest for the most energetic electrons, for which $|E|$ is equal to the work function ϕ of the metal.

Using this result in Equation 7.10 gives the transmission coefficient for field emission as

Transmission coefficient for field emission

$$T(E) \approx \exp\left(\left\{-\frac{4\sqrt{2m}\,|E|^{3/2}}{3e\hbar}\right\}\frac{1}{\mathcal{E}}\right) \tag{7.11}$$

The strong dependence of T on electron energy E in the bulk is evident from this expression. It is also apparent that the quantity in curly brackets must have the dimensions of electric field and represents a characteristic field strength—say, $\mathcal{E}_c$—for field emission:

$$\mathcal{E}_c = \frac{4\sqrt{2m}|E|^{3/2}}{3e\hbar} \tag{7.12}$$

The escape probability is largest for the most energetic electrons; these are the ones most loosely bound and for which $|E| = \phi$, the work function of the

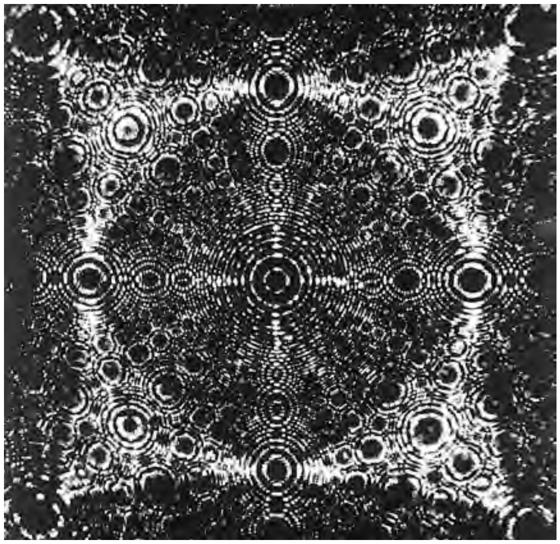

Figure 7.8 Field emission microscope image of the surface of a crystalline platinum alloy with a magnification of 3,000,000×. Individual atoms can be seen on surface layers using this technique. *(Manfred Kage/Peter Arnold, Inc.)*

metal. For $|E| = \phi = 4.0$ eV, a typical value for many metals, we calculate the characteristic field strength to be $\mathcal{E}_c = 5.5 \times 10^{10}$ V/m, a strong field by laboratory standards. Measurable emission occurs even with much weaker fields, however, since the emission *rate* depends on the product of the transmission coefficient and the number of electrons per second that collide with the barrier. This collision frequency is quite high for a bulk sample containing something like 10^{22} electrons per cubic centimeter, and values in excess of 10^{30} collisions per second per square centimeter are not uncommon (see Problem 18)! In this way field emission rates on the order of 10^{10} electrons per second (currents of about 1 nA) can be realized with applied fields as small as $\mathcal{E}_c/50$, or about 10^9 V/m.

EXAMPLE 7.5 Tunneling in a Parallel-Plate Capacitor

Estimate the leakage current due to tunneling that passes across a parallel-plate capacitor charged to a potential difference of 10 kV. Take the plate separation to be $d = 0.010$ mm and the plate area to be $A = 1.0$ cm^2.

Solution The number of electrons per second impinging on the plate surface from the bulk is the collision frequency f, about 10^{30} per second per square centimeter for most metals. Of these, only the fraction given by the transmission coefficient T can tunnel through the potential barrier in the gap to register as a current through the device. Thus, the electron emission rate for a plate of area 1 cm^2 is

$$\lambda = fT(E) = 1.0 \times 10^{30} \exp(-\mathcal{E}_c/\mathcal{E})$$

The electric field $\mathcal{E}$ in the gap is 10 kV/0.010 mm = 1.0×10^9 V/m. Using this and $\mathcal{E}_c = 5.5 \times 10^{10}$ V/m gives for the exponential $\exp\{-55\} = 1.30 \times 10^{-24}$ and an emission rate of $\lambda = 1.30 \times 10^6$ electrons per second. Since each electron carries a charge $e = 1.60 \times 10^{-19}$ C, the tunneling current is

$$I = 2.1 \times 10^{-13} \text{ A} = 0.21 \text{ pA}$$

α Decay

The decay of radioactive elements with the emission of α particles (helium nuclei composed of two protons and two neutrons) was among the long-standing puzzles to which the fledgling field of wave mechanics was first applied shortly after its inception in 1926. That α particles are a disintegration product of such species as radium, thorium, and uranium was well documented as early as 1900, but certain features of this decay remained a mystery, finally unraveled in 1928 in the now-classic works of George Gamow and R. W. Gurney and E. U. Condon. Their contribution was to recognize that the newly discovered tunnel effect lay behind the two most puzzling aspects of α decay:

- All α particles emitted from any one source have nearly the same energy and, for all known emitters, emerge with kinetic energies in the same narrow range, from about 4 to 9 MeV.
- In contrast to the uniformity of energies, the half-life of the emitter (time taken for half of the emitting substance to decay) varies over an enormous range—more than 20 orders of magnitude!—according to the emitting element (Table 7.1).

For instance, alphas emerge from the element thorium with kinetic energy equal to 4.05 MeV, only a little less than half as much as the alphas emitted from polonium (8.95 MeV). Yet the half-life of thorium is 1.4×10^{10} years, compared with only 3.0×10^{-7} *seconds* for the half-life of polonium!

Gamow attributed this striking behavior to a preformed α particle rattling around within the nucleus of the radioactive (parent) element, eventually tunneling through the potential barrier to escape as a detectable decay product (Fig. 7.9a). While inside the parent nucleus, the α is virtually free, but nonetheless confined to the nuclear potential well by the nuclear force. Once outside the nucleus, the α particle experiences only the Coulomb repulsion of the emitting (daughter) nucleus. (The nuclear force on the α outside the nucleus is insignificant due to its extremely short range, $\approx 10^{-15}$ m.) Figure 7.9b shows the potential-energy diagram for the α particle as a function of distance r from the emitting nucleus. The nuclear radius R is about 10^{-14} m, or 10 fm [note that 1 fm (fermi) = 10^{-15} m] for heavy nuclei[2]; beyond this there is only the energy of Coulomb repulsion, $U(r) = kq_1q_2/r$, between the doubly charged α

Table 7.1 Characteristics of Some Common α Emitters

Element	α Energy	Half-Life*
$^{212}_{84}$Po	8.95 MeV	2.98×10^{-7} s
$^{240}_{96}$Cm	6.40 MeV	27 days
$^{226}_{88}$Ra	4.90 MeV	1.60×10^{3} yr
$^{232}_{90}$Th	4.05 MeV	1.41×10^{10} yr

*Note that half-lives range over 24 orders of magnitude when α energy changes by a factor of 2.

[2]The fermi (fm) is a unit of distance commonly used in nuclear physics.

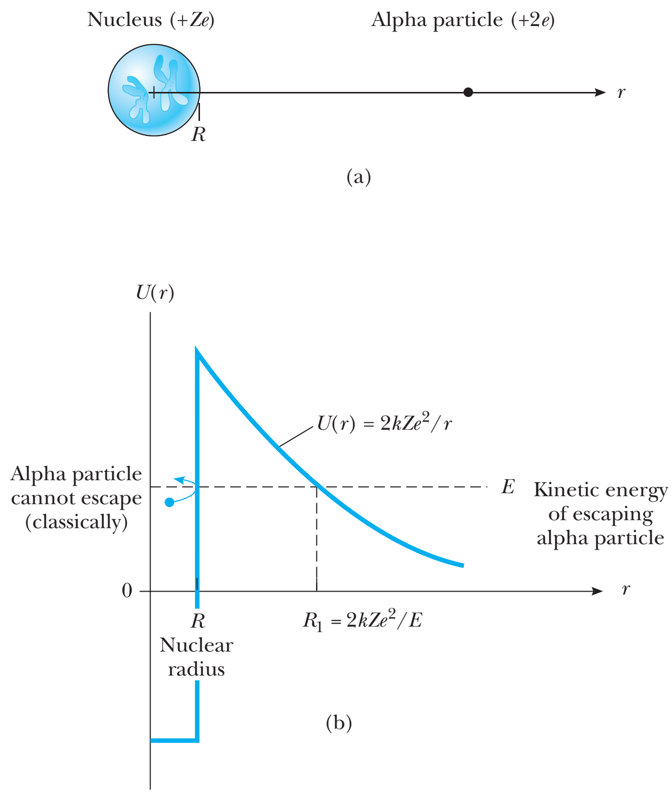

Figure 7.9 (a) α decay of a radioactive nucleus. (b) The potential energy seen by an α particle emitted with energy E. R is the nuclear radius, about 10^{-14} m, or 10 fm. α particles tunneling through the potential barrier between R and R_1 escape the nucleus to be detected as radioactive decay products.

($q_1 = +2e$) and a daughter nucleus with atomic number Z ($q_2 = +Ze$). Classically, even a 9-MeV α particle initially bound to the nucleus would have insufficient energy to overcome the Coulomb barrier ($\approx$30 MeV high) and escape. But the α particle, with its wave attributes, may tunnel *through* the barrier to appear on the outside. The total α particle energy E inside the nucleus becomes the observed kinetic energy of the emerging α once it has escaped. **It is the sensitivity of the tunneling rate to small changes in particle energy that accounts for the wide range of half-lives observed for α emitters.**

Tunneling through the Coulomb barrier

The tunneling probability and associated decay rate are calculated in much the same way as for field emission, apart from the fact that the barrier shape now is Coulombic, rather than triangular. The details of this calculation are given in Example 13.9 (Chapter 13), with the result

Transmission coefficient for α particles of an unstable nucleus

$$T(E) = \exp\left\{-4\pi Z\sqrt{\frac{E_0}{E}} + 8\sqrt{\frac{ZR}{r_0}}\right\} \tag{7.13}$$

In this expression, $r_0 = \hbar^2/m_\alpha ke^2$ is a kind of "Bohr" radius for the α particle. The mass of the α particle is $m_\alpha = 7295m_e$, so r_0 has the value $a_0/7295 = 7.25 \times 10^{-5}$ Å, or 7.25 fm. The length r_0, in turn, defines a convenient energy unit E_0 analogous to the Rydberg in atomic physics:

$$E_0 = \frac{ke^2}{2r_0} = \left(\frac{ke^2}{2a_0}\right)\left(\frac{a_0}{r_0}\right) = (13.6 \text{ eV})(7295) = 0.0993 \text{ MeV}$$

To obtain decay rates, $T(E)$ must be multiplied by the number of collisions per second that an α particle makes with the nuclear barrier. This collision frequency f is the reciprocal of the transit time for the α particle crossing the nucleus, or $f = v/2R$, where v is the speed of the α particle inside the nucleus. In most cases, f is about 10^{21} collisions per second (see Problem 17). The decay rate λ (the probability of α emission per unit time) is then

$$\lambda = fT(E) \approx 10^{21} \exp\{-4\pi Z\sqrt{E_0/E} + 8\sqrt{Z(R/r_0)}\}$$

The reciprocal of λ has dimensions of time and is related to the half-life of the emitter $t_{1/2}$ as

$$t_{1/2} = \frac{\ln 2}{\lambda} = \frac{0.693}{\lambda} \tag{7.14}$$

EXAMPLE 7.6 Estimating the Half-lives of Thorium and Polonium

Using the tunneling model just developed, estimate the half-lives for α decay of the radioactive elements thorium and polonium. The energy of the ejected alphas is 4.05 MeV and 8.95 MeV, respectively, and the nuclear size is about 9.00 fm in both cases.

Solution For thorium ($Z = 90$), the daughter nucleus has atomic number $Z = 88$, corresponding to the element radium. Using $E = 4.05$ MeV and $R = 9.00$ fm, we find for the transmission factor $T(E)$ in Equation 7.13

$$\exp\{-4\pi(88)\sqrt{(0.0993/4.05)} + 8\sqrt{88(9.00/7.25)}\} = \exp\{-89.542\} = 1.3 \times 10^{-39}$$

Taking $f = 10^{21}$ Hz, we obtain for the decay rate the value $\lambda = 1.29 \times 10^{-18}$ alphas per second. The associated half-life is, from Equation 7.14,

$$t_{1/2} = \frac{0.693}{1.3 \times 10^{-18}} = 5.4 \times 10^{17} \text{ s} = 1.7 \times 10^{10} \text{ yr}$$

which compares favorably with the actual value for thorium, 1.4×10^{10} yr.

If polonium ($Z = 84$) is the radioactive species, the daughter element is lead, with $Z = 82$. Using for the disintegration energy $E = 8.95$ MeV, we obtain for the transmission factor

$$\exp\{-4\pi(82)\sqrt{(0.0993/8.95)} + 8\sqrt{82(9.00/7.25)}\} = \exp\{-27.825\} = 8.2 \times 10^{-13}$$

Assuming f is unchanged at 10^{21} collisions per second, we get for this case $\lambda = 8.2 \times 10^8$ alphas per second and a half-life

$$t_{1/2} = \frac{0.693}{8.2 \times 10^8} = 8.4 \times 10^{-10} \text{ s}$$

The measured half-life of polonium is 3.0×10^{-7} s.

Given the crudeness of our method, both estimates should be considered satisfactory. Further, the calculations show clearly how a factor of only 2 in disintegration energy leads to half-lives differing by more than 26 orders of magnitude!

The radioactive decay process also can be understood in terms of the time evolution of a nonstationary state, in this case one representing the α particle initially confined to the parent nucleus. Solving the Schrödinger equation for the time-dependent waveform in this instance is complicated, making numerical studies the option of choice here. The interested reader is referred to our companion Web site for further details and a fully quantum-mechanical simulation of α decay from an unstable nucleus. Go to http://info.brookscole.com/mp3e, select QMTools Simulations → Leaky Wells (Tutorial) and follow the on-site instructions.

Ammonia Inversion

The "inversion" of the ammonia molecule is another example of tunneling, this time for an entire atom. The equilibrium configuration of the ammonia (NH_3) molecule is shown in Figure 7.10a: The nitrogen atom is situated at the apex of a pyramid whose base is the equilateral triangle formed by the three hydrogen atoms. But this equilibrium is not truly stable; indeed, there is a second equilibrium position for the nitrogen atom on the opposite side of the plane formed by the hydrogen atoms. With its two equilibrium locations, the nitrogen atom of the ammonia molecule constitutes a **double oscillator,** which can be modeled by using the potential shown in Figure 7.10b. A nitrogen atom initially located on one side of the symmetry plane will not remain there indefinitely, since there is some probability that it can tunnel through the oscillator barrier to emerge on the other side. When this occurs, the molecule becomes *inverted* (Fig. 7.10c). But the process does not stop there; the nitrogen atom, now on the opposite side of the symmetry plane, has a probability of tunneling back through the barrier to take up its original position! The molecule does not just undergo one inversion, but flip-flops repeatedly, alternating between the two classical equilibrium configurations. The "flopping" frequency is fixed by the tunneling rate and turns out to be quite high, on the order of 10^{10} Hz (microwave range of the electromagnetic spectrum)!

Double oscillator representation of the ammonia molecule

We can estimate the tunneling probability for inversion using Equation 7.10. The double oscillator potential of Figure 7.10b is described by the potential energy function

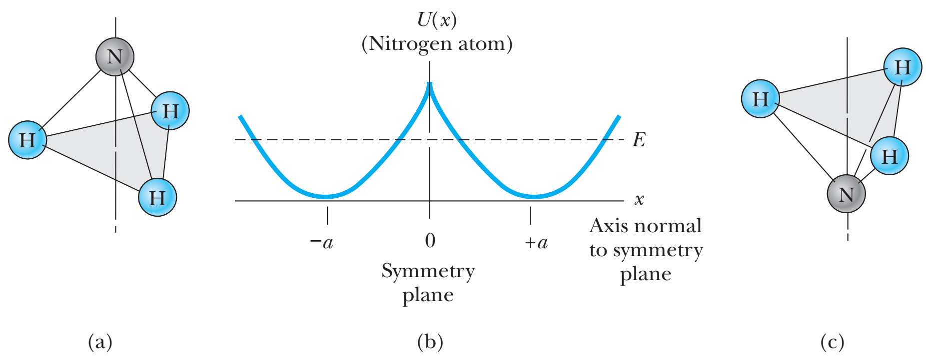

Figure 7.10 (a) The ammonia molecule NH_3. At equilibrium, the nitrogen atom is situated at the apex of a pyramid whose base is the equilateral triangle formed by the three hydrogen atoms. By symmetry, a second equilibrium configuration exists for the nitrogen atom on the opposite side of the plane formed by the hydrogen atoms. (b) The potential energy seen by the nitrogen atom along a line perpendicular to the symmetry plane. The two equilibrium points at $-a$ and $+a$ give rise to the double oscillator potential shown. A nitrogen atom with energy E can tunnel back and forth through the barrier from one equilibrium point to the other, with the result that the molecule alternates between the normal configuration in (a) and the inverted configuration shown in (c).

$$U(x) = \tfrac{1}{2}M\omega^2(|x| - a)^2 \tag{7.15}$$

with ω the classical frequency of vibration for the nitrogen atom around either of the equilibrium points $x = \pm a$. We suppose the nitrogen atom possesses the minimum energy of vibration, $E = \frac{1}{2}\hbar\omega$. There are four classical turning points for which $U(x) = E$ (see Fig. 7.10b); the limits for the tunneling integral are the pair closest to $x = 0$, and these are given by $x = \pm(a - A)$, where A is the vibration amplitude for the nitrogen atom in a single oscillator well. The vibration amplitude A is found from energy conservation by recognizing that here all the energy is in potential form: $\frac{1}{2}\hbar\omega = \frac{1}{2}M\omega^2A^2$, or

$$A = \sqrt{\frac{\hbar}{M\omega}} \tag{7.16}$$

Since the tunneling integral is symmetric about $x = 0$, we may write it as

$$\frac{2}{\hbar}\sqrt{2m}\int_{-(a-A)}^{a-A}\sqrt{U(x) - E}\,dx = \frac{4}{A^2}\int_0^{a-A}\sqrt{(x-a)^2 - A^2}\,dx$$

where $U(x)$ and E have been expressed in terms of A, using Equation 7.16. The integral on the right can be evaluated in terms of hyperbolic functions,[3] with the result

$$\frac{4}{A^2}\int_0^{a-A}\sqrt{(x-a)^2 - A^2}\,dx = \sinh(2y_0) - 2y_0$$

where y_0 is defined by the relation $\cosh(y_0) = a/A$. The transmission coefficient is then

$$T = e^{-[\sinh(2y_0) - 2y_0]} \tag{7.17}$$

To get the tunneling rate λ (and its reciprocal—the tunneling time), we must multiply T by the frequency with which the nitrogen atom collides with the potential barrier. For an atom vibrating about its equilibrium position, this is the vibration frequency $f = \omega/2\pi$. From Equation 7.16, we see that f is related to the vibration amplitude as $f = \hbar/2\pi MA^2$.

The tunneling rate depends sensitively on the values chosen for a and A. For the equilibrium distance from the symmetry plane, we take $a = 0.38$ Å, an experimental value obtained from x-ray diffraction measurements.[4] The vibration amplitude A is not directly observable, but its value can be calculated from $U(0)$, the height of the potential barrier at $x = 0$, which is known to be 0.25690 eV. Using Equations 7.15 and 7.16, and taking $M = 14$ u for the mass of the nitrogen atom, we find

$$A = \left(\frac{\hbar^2a^2}{2MU(0)}\right)^{1/4} = \left(\frac{(1.973\text{ keV}\cdot\text{Å}/c)^2(0.38\text{Å})^2}{2(14)(931.50\times10^3\text{ keV}/c^2)(0.2569\times10^{-3}\text{ keV})}\right)^{1/4}$$
$$= 0.096\text{Å}$$

[3] Introduce a new integration variable y with the substitution $x - a = -A\cosh(y)$, and use the properties of the hyperbolic cosine and sine functions, $\cosh(y) = \frac{1}{2}(e^y + e^{-y})$, $\sinh(y) = \frac{1}{2}(e^y - e^{-y})$, to obtain the final form.

[4] B. H. Bransden and C. J. Joachain, *Physics of Atoms and Molecules*, New York, John Wiley and Sons, Inc., 1983, p. 456.

This underestimates the true value for A because we have (incorrectly) identified M as the mass of the nitrogen atom. In fact, M should be the *reduced mass* of the nitrogen–hydrogen group, about 2.47 u.[5] With this correction, we find $A = 0.148$ Å and a tunneling rate $\lambda = fT \approx 2.4 \times 10^{12}$ Hz. The observed tunneling rate, 2.4×10^{10} Hz, suggests a somewhat smaller value for A. By trial and error, we find the actual tunneling rate is reproduced with $A = 0.125$ Å, still a reasonable figure for the vibration amplitude of the nitrogen atom in the ammonia molecule.

Notice that because of tunneling, the nitrogen atom on one side of the symmetry plane or the other does *not* constitute a stationary state of the ammonia molecule, since the probability for finding it there changes over time. In fact, the flopping behavior stems from a simple combination of two stationary states of nearly equal energy for the nitrogen atom in this environment. Such superpositions of closely spaced (in energy) stationary states have applications that transcend this one example and are the subject of a computer-based tutorial available at our companion Web site. For more information, go to http://info.brookscole.com/mp3e, select QMTools Simulations → Two-Center Potentials (Tutorial), and follow the on-site instructions.

Since the flopping frequency is in the microwave range, the ammonia molecule can serve as an amplifier for microwave radiation. The **ammonia maser** operates on this principle. Because of the small energy difference between the ground and first excited states of the ammonia molecule, ammonia vapor at room temperature has roughly equal numbers of molecules in both states. Having opposite electric dipole moments, these states are easily separated by passing the vapor through a nonuniform electric field. In this way, ammonia vapor can be produced with the unusually large concentrations of excited molecules needed to create the population inversion necessary for maser operation. A spontaneous deexcitation to the ground state of one molecule releases a (microwave) photon, which, in turn, induces other molecules to deexcite. The result—much like a chain reaction—produces a photon cascade: an intense burst of coherent microwave radiation. The operation of masers and lasers is discussed in more detail in Chapter 12 and on our website at http://info.brookscole.com/mp3e.

Decay of Black Holes

Once inside the event horizon, nothing—not even light—can escape the gravitational pull of a black hole.[6] That was the view held until 1974, when the brilliant British astrophysicist Stephen Hawking proposed that black holes are indeed radiant objects, emitting a variety of particles by a mechanism involving tunneling through the (gravitational) potential barrier surrounding the black hole. The thickness of this barrier is proportional to the size of the black hole, so that the likelihood of a tunneling event initially may be extremely small. As the black hole emits particles, however, its mass and size steadily

[5]In this mode of vibration, all three hydrogen atoms move in unison as if they were a single object with mass 3 u. The reduced mass refers to the pair consisting of this total mass and the mass of the nitrogen atom (14 u).

[6]A brief introduction to black holes is found in Clifford Will's essay "The Renaissance of General Relativity" on our companion Web site.

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decrease, making it easier for more particles to tunnel out. In this way emission continues at an ever-increasing rate, until eventually the black hole radiates itself out of existence in an explosive climax! Thus, Hawking's scenario leads inexorably to the decay and eventual demise of any black hole.

Calculations indicate that a black hole with the mass of our Sun would survive against decay by tunneling for about 10^{66} years. On the other hand, a black hole with the mass of only a billion tons and roughly the size of a proton (such mini black holes are believed to have been formed just after the Big Bang origin of the Universe) should have almost completely evaporated in the 10 billion years that have elapsed since the time of creation, and black holes a few times heavier should still be evaporating strongly. A large portion of the energy emitted by such holes would be in the form of gamma rays. Indeed, gamma rays from interstellar space have been observed, but in quantities and with properties that are readily explained in other ways. Currently there is no compelling observational evidence of black-hole evaporation in the Universe today.

SUMMARY

For potentials representing barriers, the stationary states are not localized, but extend throughout the entire space in a manner that describes particle scattering. When a matter wave encounters a potential barrier, part of the wave is reflected by the barrier and part is transmitted through the barrier. In particle language, an object colliding with the barrier does not predictably rebound or penetrate, but can only be assigned probabilities for reflection and transmis-