## More

In order for interesting things to happen in systems with quantized energies, the probability density must change in time. Only in this way can energy be emitted or absorbed by the system. *Transitions Between Energy States* on the home page (www.whfreeman.com/tiplermodernphysics5e) describes the process and applies it to the emission of light from an atom. See also Equations 6-52*a–e* and Figure 6-16 here.

# 6-5 The Simple Harmonic Oscillator

One of the problems solved by Schrödinger in the second of his six famous papers was that of the simple harmonic oscillator potential, given by

$$V(x) = \frac{1}{2}Kx^2 = \frac{1}{2}m\omega^2x^2$$

where $K$ is the force constant and $\omega$ the angular frequency of vibration defined by $\omega = (K/m)^{1/2} = 2\pi f$. The solution of the Schrödinger equation for this potential is particularly important, as it can be applied to such problems as the vibration of molecules in gases and solids. This potential energy function is shown in Figure 6-17, with a possible total energy $E$ indicated.

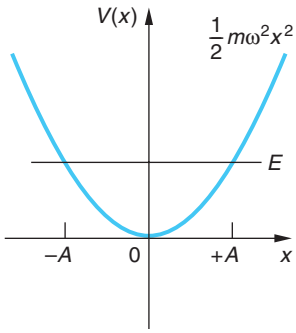



Figure 6-17 Potential energy function for a simple harmonic oscillator. Classically, the particle is confined between the "turning points" $-A$ and $+A$.

In classical mechanics, a particle in such a potential is in equilibrium at the origin $x = 0$, where $V(x)$ is minimum and the force $F_x = -dV/dx$ is zero. If disturbed, the particle will oscillate back and forth between $x = -A$ and $x = +A$, the points at which the kinetic energy is zero and the total energy is just equal to the potential energy. These points are called the classical turning points. The distance $A$ is related to the total energy $E$ by

$$E = \frac{1}{2}m\omega^2A^2 \qquad \textbf{6-53}$$

Classically, the probability of finding the particle in $dx$ is proportional to the time spent in $dx$, which is $dx/v$. The speed of the particle can be obtained from the conservation of energy:

$$\frac{1}{2}mv^2 + \frac{1}{2}m\omega^2x^2 = E$$

The classical probability is thus

$$P_c(x)\,dx \propto \frac{dx}{v} = \frac{dx}{\sqrt{(2/m)\left(E - \frac{1}{2}m\omega^2x^2\right)}} \qquad \textbf{6-54}$$

Any value of the energy $E$ is possible. The lowest energy is $E = 0$, in which case the particle is at rest at the origin.

The Schrödinger equation for this problem is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + \frac{1}{2}m\omega^2x^2\psi(x) = E\psi(x) \qquad \textbf{6-55}$$

The mathematical techniques involved in solving this type of differential equation are standard in mathematical physics but unfamiliar to most students at this level. We will, therefore, discuss the problem qualitatively. We first note that since the potential is symmetric about the origin $x = 0$, we expect the probability distribution function $|\psi(x)|^2$ also to be symmetric about the origin, i.e., to have the same value at $-x$ as at $+x$.

$$|\psi(-x)|^2 = |\psi(x)|^2$$

The wave function $\psi(x)$ must then be either symmetric $\psi(-x) = +\psi(x)$ or antisymmetric $\psi(-x) = -\psi(x)$. We can therefore simplify our discussion by considering positive $x$ only and find the solutions for negative $x$ by symmetry. (The symmetry of $\Psi$ is discussed further in the Exploring section, Parity; see page 250.)

Consider some value of total energy $E$. For $x$ less than the classical turning point $A$ defined by Equation 6-53, the potential energy $V(x)$ is less than the total energy $E$, whereas for $x > A$, $V(x)$ is greater than $E$. Our discussion in Section 6-3 applies directly to this problem. For $x < A$, the Schrödinger equation can be written

$$\psi''(x) = -k^2\psi(x)$$

where

$$k^2 = \frac{2m}{\hbar^2}[E - V(x)]$$

and $\psi(x)$ curves toward the axis and oscillates. For $x > A$, the Schrödinger equation becomes

$$\psi''(x) = +\alpha^2\psi(x)$$

with

$$\alpha^2 = \frac{2m}{\hbar^2}[V(x) - E]$$

and $\psi(x)$ curves away from the axis. Only certain values of $E$ will lead to solutions that are well behaved, i.e., that approach zero as $x$ approaches infinity. The allowed values of $E$ for the simple harmonic oscillator must be determined by solving the Schrödinger equation; in this case they are given by

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, \ldots \qquad \textbf{6-56}$$

Thus, the ground-state energy is $\frac{1}{2}\hbar\omega$ and the energy levels are equally spaced, each excited state being separated from the levels immediately adjacent by $\hbar\omega$.

The wave functions of the simple harmonic oscillator in the ground state and in the first two excited states ($n = 0$, $n = 1$, and $n = 2$) are sketched in Figure 6-18. The ground-state wave function has the shape of a Gaussian curve, and the lowest energy $E = \frac{1}{2}\hbar\omega$ is the minimum energy consistent with the uncertainty principle.

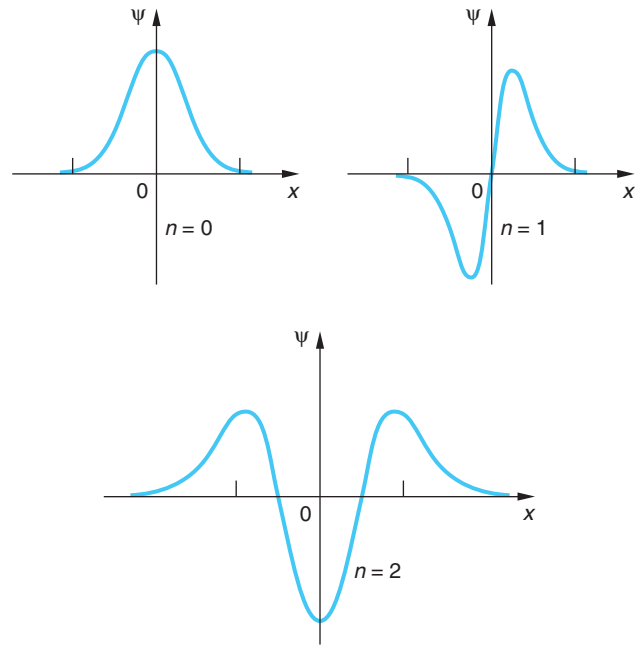



Figure 6-18 Wave functions for the ground state and the first two excited states of the simple harmonic oscillator potential, the states with $n = 0$, 1, and 2.

The allowed solutions to the Schrödinger equation, the wave functions for the simple harmonic oscillator, can be written

$$\psi_n(x) = C_n e^{-m\omega x^2/2\hbar} H_n(x) \qquad \textbf{6-57}$$

where the constants $C_n$ are determined by normalization and the functions $H_n(x)$ are polynomials of order $n$ called the Hermite polynomials.[13] The solutions for $n = 0$, 1, and 2 (see Figure 6-18) are

$$\begin{aligned}
\psi_0(x) &= A_0 e^{-m\omega x^2/2\hbar} \\
\psi_1(x) &= A_1 \sqrt{\frac{m\omega}{\hbar}}\, x e^{-m\omega x^2/2\hbar} \qquad \textbf{6-58} \\
\psi_2(x) &= A_2 \left(1 - \frac{2m\omega x^2}{\hbar}\right) e^{-m\omega x^2/2\hbar}
\end{aligned}$$

Molecules vibrate as harmonic oscillators. Measuring vibration frequencies (see Chapter 9) enables determination of force constants, bond strengths, and properties of solids.

Notice that for even values of $n$, the wave functions are symmetric about the origin; for odd values of $n$, they are antisymmetric. In Figure 6-19 the probability distributions $\psi_n^2(x)$ are sketched for $n = 0$, 1, 2, 3, and 10 for comparison with the classical distribution.

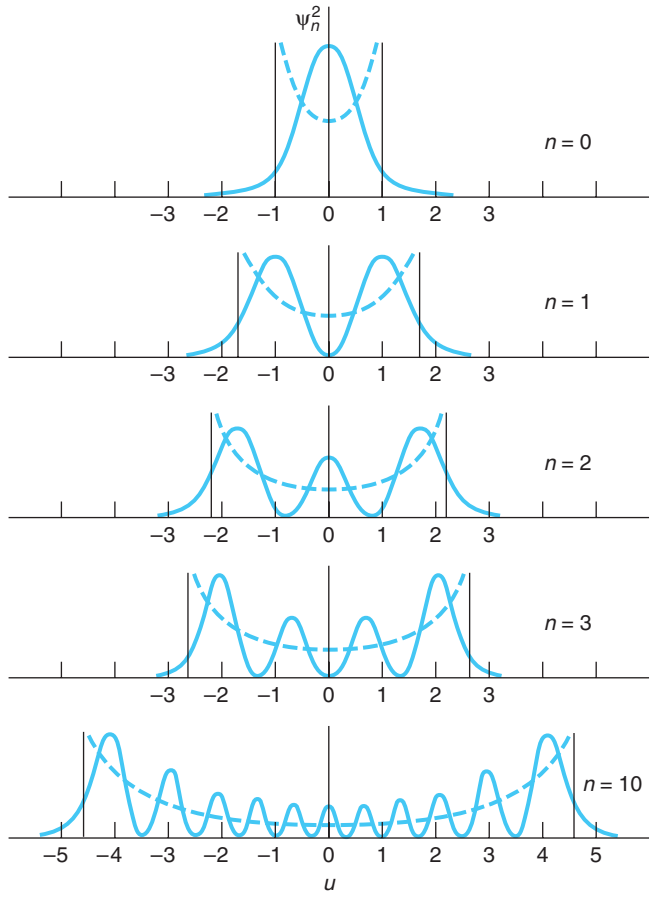



Figure 6-19 Probability density $\psi_n^2$ for the simple harmonic oscillator plotted against the dimensionless variable $u = (m\omega/\hbar)^{1/2}x$, for $n = 0$, 1, 2, 3, and 10. The dashed curves are the classical probability densities for the same energy, and the vertical lines indicate the classical turning points $x = \pm A$.

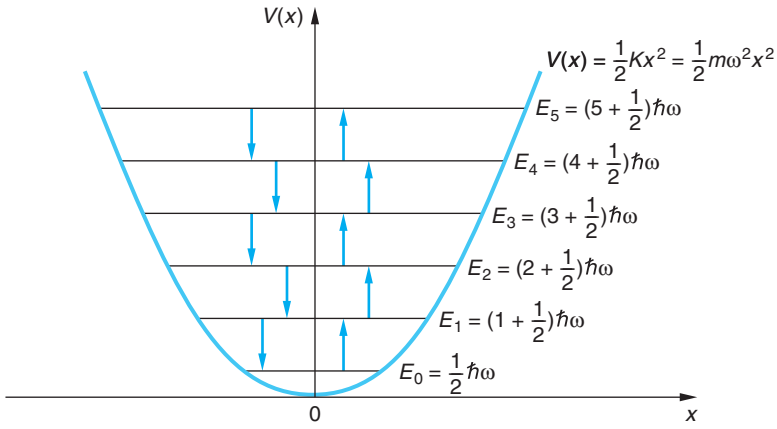



Figure 6-20 Energy levels in the simple harmonic oscillator potential. Transitions obeying the selection rule $\Delta n = \pm 1$ are indicated by the arrows (those pointing up indicate absorption). Since the levels have equal spacing, the same energy $\hbar\omega$ is emitted or absorbed in all allowed transitions. For this special potential, the frequency of the emitted or absorbed photon equals the frequency of oscillation, as predicted by classical theory.

A property of these wave functions that we will state without proof is that

$$\int_{-\infty}^{+\infty} \psi_n^* x \psi_m \, dx = 0 \quad \text{unless} \quad n = m \pm 1 \qquad \textbf{6-59}$$

This property places a condition on transitions that may occur between allowed states. This condition, called a *selection rule*, limits the amount by which $n$ can change for (electric dipole) radiation emitted or absorbed by a simple harmonic oscillator:

The quantum number of the final state must be 1 less than or 1 greater than that of the initial state.

This selection rule is usually written

$$\Delta n = \pm 1 \qquad \textbf{6-60}$$

Since the difference in energy between two successive states is $\hbar\omega$, this is the energy of the photon emitted or absorbed in an electric dipole transition. The frequency of the photon is therefore equal to the classical frequency of the oscillator, as was assumed by Planck in his derivation of the blackbody radiation formula. Figure 6-20 shows an energy level diagram for the simple harmonic oscillator, with the allowed energy transitions indicated by vertical arrows.

## More

Solution of the Schrödinger equation for the simple harmonic oscillator (Equation 6-55) involves some rather advanced differential equation techniques. However, a simpler exact solution is also possible using an approach invented by Schrödinger himself that we will call *Schrödinger's Trick*. With the authors' thanks to Wolfgang Lorenzon for bringing it to our attention, we include it on the home page www.whfreeman.com/tiplermodernphysics5e so that you, too, will know the trick.

## EXPLORING
### Parity

We made a special point of arranging the simple harmonic oscillator potential symmetrically about $x = 0$ (see Figure 6-17), just as we had done with the finite square well in Figure 6-8*b* and will do with various other potentials in later discussions. The usual purpose in each case is to emphasize the symmetry of the physical situation and to simplify the mathematics. Notice that arranging the potential $V(x)$ symmetrically about the origin means that $V(x) = V(-x)$. This means that the Hamiltonian operator $H_{op}$, defined in Equation 6-51, is unchanged by a transformation that changes $x \longrightarrow -x$. Such a transformation is called a *parity operation* and is usually denoted by the operator $P$. Thus, if $\psi(x)$ is a solution of the Schrödinger equation

$$H_{op}\psi(x) = E\psi(x) \qquad \textbf{6-52}$$

then a parity operation $P$ leads to

$$H_{op}\psi(-x) = E\psi(-x)$$

and $\psi(-x)$ is also a solution to the Schrödinger equation and corresponds to the same energy. When two (or more) wave functions are solutions corresponding to the same value of the energy $E$, that level is referred to as *degenerate*. In this case, where two wave functions, $\psi(x)$ and $\psi(-x)$, are both solutions with energy $E$, we call the energy level doubly degenerate.

It should be apparent from examining the two equations above that $\psi(x)$ and $\psi(-x)$ can differ at most by a multiplicative constant $C$; i.e.,

$$\psi(x) = C\psi(-x) \qquad \psi(-x) = C\psi(x)$$

or

$$\psi(x) = C\psi(-x) = C^2\psi(x)$$

from which it follows that $C = \pm 1$. If $C = 1$, $\psi(x)$ is an even function, i.e., $\psi(-x) = \psi(x)$. If $C = -1$, then $\psi(x)$ is an odd function, i.e., $\psi(-x) = -\psi(x)$. Parity is used in quantum mechanics to describe the symmetry properties of wave functions under a reflection of the *space* coordinates in the origin, i.e., under a parity operation. The terms even and odd parity describe the symmetry of the wave functions, not whether the quantum numbers are even or odd. We will have more on parity in Chapter 12.

## 6-6 Reflection and Transmission of Waves

Up to this point, we have been concerned with bound-state problems in which the potential energy is larger than the total energy for large values of $x$. In this section, we will consider some simple examples of unbound states for which $E$ is greater than $V(x)$ as $x$ gets larger in one or both directions. For these problems $d^2\psi(x)/dx^2$ and $\psi(x)$ have opposite signs for those regions of $x$ where $E > V(x)$, so $\psi(x)$ in those regions curves toward the axis and does not become infinite at large values of $|x|$. Any value of $E$ is allowed. Such wave functions are not normalizable since $\psi(x)$ does not approach zero as $x$ goes to infinity in at least one direction and, as a consequence,

$$\int_{-\infty}^{+\infty} |\psi(x)|^2\, dx \longrightarrow \infty$$

A complete solution involves combining infinite plane waves into a wave packet of finite width. The resulting finite packet is normalizable. However, for our purposes it is sufficient to note that the integral above is bounded between the limits $a$ and $b$, provided only that $|b - a| < \infty$. Such wave functions are most frequently encountered, as we are about to do, in the scattering of beams of particles from potentials, so it is usual to normalize such wave functions in terms of the density of particles ρ in the beam. Thus,

$$\int_a^b |\psi(x)|^2\, dx = \int_a^b \rho\, dx = \int_a^b dN = N$$

where $dN$ is the number of particles in the interval $dx$ and $N$ is the number of particles in the interval $(b - a)$.[14] The wave nature of the Schrödinger equation leads, even so, to some very interesting consequences.

## Step Potential

Consider a region in which the potential energy is the step function

$$V(x) = 0 \quad \text{for} \quad x < 0$$
$$V(x) = V_0 \quad \text{for} \quad x > 0$$

as shown in Figure 6-21. We are interested in what happens when a beam of particles, each with the same total energy $E$, moving from left to right encounters the step.

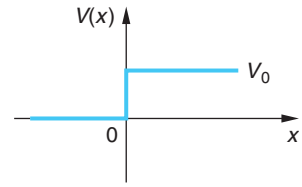



Figure 6-21 Step potential. A classical particle incident from the left, with total energy $E$ greater than $V_0$, is always transmitted. The potential change at $x = 0$ merely provides an impulsive force that reduces the speed of the particle. However, a wave incident from the left is partially transmitted and partially reflected because the wavelength changes abruptly at $x = 0$.

The classical answer is simple. For $x < 0$, each particle moves with speed $v = (2E/m)^{1/2}$. At $x = 0$, an impulsive force acts on it. If the total energy $E$ is less than $V_0$, the particle will be turned around and will move to the left at its original speed; that is, it will be reflected by the step. If $E$ is greater than $V_0$, the particle will continue moving to the right but with reduced speed, given by $v = [2(E - V_0)/m]^{1/2}$. We might picture this classical problem as a ball rolling along a level surface and coming to a steep hill of height $y_0$, given by $mgy_0 = V_0$. If its original kinetic energy is less than $V_0$, the ball will roll partway up the hill and then back down and to the left along the level surface at its original speed. If $E$ is greater than $V_0$, the ball will roll up the hill and proceed to the right at a smaller speed.

The quantum-mechanical result is similar to the classical one for $E < V_0$ but quite different when $E > V_0$, as in Figure 6-22*a*. The Schrödinger equation in each of the two space regions shown in the diagram is given by

**Region I**

$$(x < 0) \qquad \frac{d^2\psi(x)}{dx^2} = -k_1^2\psi(x) \qquad \textbf{6-61}$$

**Region II**

$$(x > 0) \qquad \frac{d^2\psi(x)}{dx^2} = -k_2^2\psi(x) \qquad \textbf{6-62}$$

$$k_1 = \frac{\sqrt{2mE}}{\hbar} \quad \text{and} \quad k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar}$$

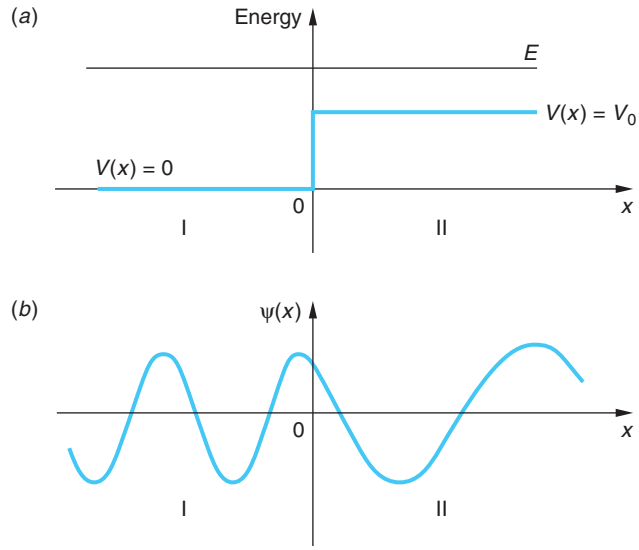



Figure 6-22 (*a*) A potential step. Particles are incident on the step from the left toward the right, each with total energy $E > V_0$. (*b*) The wavelength of the incident wave (Region I) is shorter than that of the transmitted wave (Region II). Since $k_2 < k_1$, $|C|^2 > |A|^2$; however, the transmission coefficient $T < 1$.

The general solutions are

**Region I**

$$(x < 0) \qquad \psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x} \qquad \textbf{6-63}$$

**Region II**

$$(x > 0) \qquad \psi_{II}(x) = Ce^{ik_2x} + De^{-ik_2x} \qquad \textbf{6-64}$$

Specializing these solutions to our situation where we are assuming the incident beam of particles to be moving from left to right, we see that the first term in Equation 6-63 represents that beam since multiplying $Ae^{ik_1x}$ by the time part of $\Psi(x, t)$, $e^{i\omega t}$, yields a plane wave (i.e., a beam of free particles) moving to the right. The second term, $Be^{-ik_2x}$, represents particles moving to the left in Region I. In Equation 6-64, $D = 0$ since that term represents particles incident on the potential step from the right and there are none. Thus, we have that the constant $A$ is known or at least obtainable (determined by normalization of $Ae^{ik_1x}$ in terms of the density of particles in the beam as explained above) and the constants $B$ and $C$ are yet to be found. We find them by applying the continuity condition on $\psi(x)$ and $d\psi(x)/dx$ at $x = 0$, i.e., by requiring that $\psi_I(0) = \psi_{II}(0)$ and $d\psi_I(0)/dx = d\psi_{II}(0)/dx$. Continuity of $\psi$ at $x = 0$ yields

$$\psi_I(0) = A + B = \psi_{II}(0) = C$$

or

$$A + B = C \qquad \textbf{6-65}\boldsymbol{a}$$

Continuity of $d\psi/dx$ at $x = 0$ gives

$$k_1A - k_1B = k_2C \qquad \textbf{6-65}\boldsymbol{b}$$

Solving Equations 6-65*a* and *b* for *B* and *C* in terms of *A* (see Problem 6-47), we have

$$B = \frac{k_1 - k_2}{k_1 + k_2} A = \frac{E^{1/2} - (E - V_0)^{1/2}}{E^{1/2} + (E - V_0)^{1/2}} A \qquad \textbf{6-66}$$

$$C = \frac{2k_1}{k_1 + k_2} A = \frac{2E^{1/2}}{E^{1/2} + (E - V_0)^{1/2}} A \qquad \textbf{6-67}$$

where Equations 6-66 and 6-67 give the relative amplitude of the reflected and transmitted waves, respectively. It is usual to define the coefficients of reflection $R$ and transmission $T$, the relative *rates* at which particles are reflected and transmitted, in terms of the squares of the amplitudes $A$, $B$, and $C$ as[15]

$$R = \frac{|B|^2}{|A|^2} = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 \qquad \textbf{6-68}$$

$$T = \frac{k_2}{k_1}\frac{|C|^2}{|A|^2} = \frac{4k_1k_2}{(k_1 + k_2)^2} \qquad \textbf{6-69}$$

from which it can be readily verified that

$$T + R = 1 \qquad \textbf{6-70}$$

Among the interesting consequences of the wave nature of the solutions to Schrödinger's equation, notice the following:

1. Even though $E > V_0$, $R$ is *not* 0; i.e., in contrast to classical expectations, some of the particles are reflected from the step. (This is analogous to the internal reflection of electromagnetic waves at the interface of two media.)
2. The value of $R$ depends on the difference between $k_1$ and $k_2$ but *not* on which is larger; i.e., a step down in the potential produces the same reflection as a step up of the same size.

Since $k = p/\hbar = 2\pi/\lambda$, the wavelength changes as the beam passes the step. We might also expect that the amplitude of $\psi_{II}$ will be less than that of the incident wave; however, recall that the $|\psi|^2$ is proportional to the particle density. Since particles move more slowly in Region II ($k_2 < k_1$), $|\psi_{II}|^2$ may be larger than $|\psi_I|^2$. Figure 6-22*b* illustrates these points. Figure 6-23 shows the time development of a wave packet incident on a potential step for $E > V_0$.

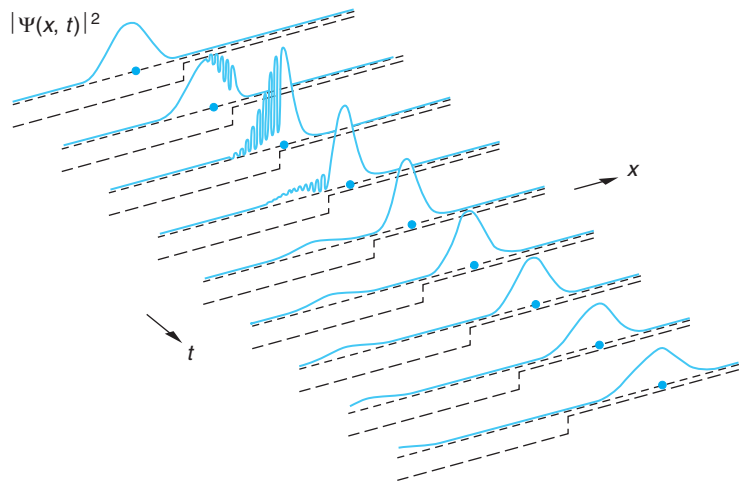



Figure 6-23 Time development of a one-dimensional wave packet representing a particle incident on a step potential for $E > V_0$. The position of a classical particle is indicated by the dot. Note that part of the packet is transmitted and part is reflected. The sharp spikes that appear are artifacts of the discontinuity in the slope of $V(x)$ at $x = 0$.

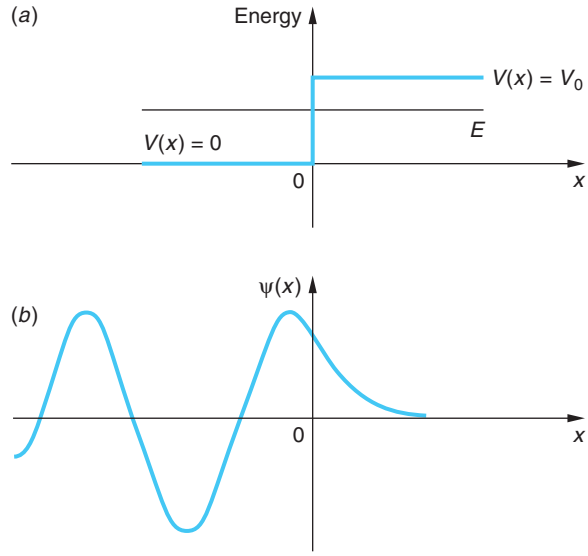



Figure 6-24 (*a*) A potential step. Particles are incident on the step from the left moving toward the right, each with total energy $E < V_0$. (*b*) The wave transmitted into region II is a decreasing exponential. However, the value of $R$ in this case is 1 and no net energy is transmitted.

Now let us consider the case shown in Figure 6-24*a*, where $E < V_0$. Classically, we expect all particles to be reflected at $x = 0$; however, we note that $k_2$ in Equation 6-64 is now an imaginary number since $E < V_0$. Thus,

$$\psi_{II}(x) = Ce^{ik_2x} = Ce^{-\alpha x} \qquad \textbf{6-71}$$

is a *real* exponential function where $\alpha = \sqrt{2m(V_0 - E)}/\hbar$. (We choose the positive root so that $\psi_{II} \to 0$ as $x \to \infty$.) This means that the numerator and denominator of the right side of Equation 6-66 are complex conjugates of each other; hence $|B|^2 = |\mathbf{A}|^2$ and $R = 1$ and $T = 0$. Figure 6-25 is a graph of both $R$ and $T$ versus energy for a potential step. In agreement with the classical prediction, all of the particles (waves) are reflected back into Region I. However, another interesting result of our solution of Schrödinger's equation is that the particle waves do not all reflect at $x = 0$.

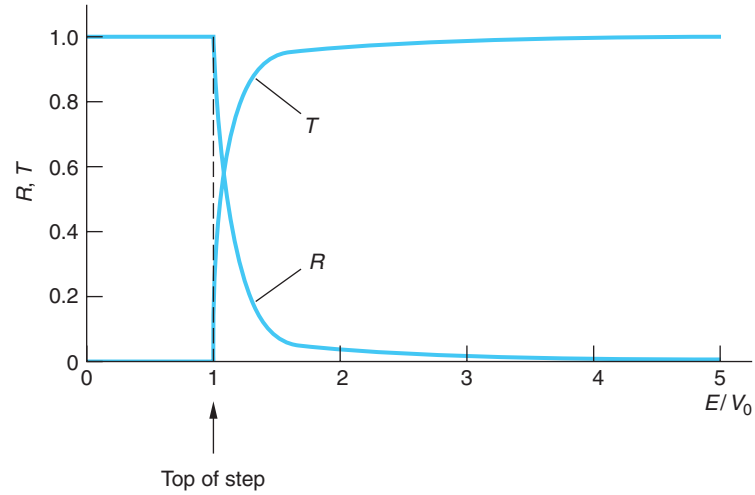



Figure 6-25 Reflection coefficient $R$ and transmission coefficient $T$ for a potential step $V_0$ high versus energy $E$ (in units of $V_0$).

Since $\psi_{II}$ is an exponential decreasing toward the right, the particle density in Region II is proportional to

$$|\psi_{II}|^2 = |C|^2 e^{-2\alpha x} \qquad \textbf{6-72}$$

Figure 6-24*b* shows the wave function for the case $E < V_0$. The wave function does not go to zero at $x = 0$ but decays exponentially, as does the wave function for the bound state in a finite square well problem. The wave penetrates slightly into the classically forbidden region $x > 0$ but eventually is completely reflected. (As discussed in Section 6-3, there is no prediction that a negative kinetic energy will be *measured* in such a region because to locate the particle in such a region introduces an uncertainty in the momentum corresponding to a minimum kinetic energy greater than $V_0 - E$.) This situation is similar to that of total internal reflection in optics.

**EXAMPLE 6-6** **Reflection from a Step with $E < V_0$** A beam of electrons, each with energy $E = 0.1\ V_0$, is incident on a potential step with $V_0 = 2$ eV. This is of the order of magnitude of the work function for electrons at the surface of metals. Graph the relative probability $|\psi|^2$ of particles penetrating the step up to a distance $x = 10^{-9}$ m, or roughly five atomic diameters.

**SOLUTION**

For $x > 0$, the wave function is given by Equation 6-71. The value of $|C|^2$ is, from Equation 6-67,

$$|C|^2 = \left| \frac{2(0.1\ V_0)^{1/2}}{(0.1\ V_0)^{1/2} + (-0.9\ V_0)^{1/2}} \right|^2 = 0.4$$

where we have taken $|A|^2 = 1$. Computing $e^{-2\alpha x}$ for several values of $x$ from 0 to $10^{-9}$ m gives, with $2\alpha = 2[2m(0.9\ V_0)]^{1/2}/\hbar$, the first two columns of the Table 6-2. Taking $e^{-2\alpha x}$ and then multiplying by $|C|^2 = 0.4$ yields $|\psi|^2$, which is graphed in Figure 6-26.

Table 6-2 $|\psi|^2$

| $x$ (m) | $2\alpha x$ | $\lvert\psi\rvert^2$ |
|---|---|---|
| 0 | 0 | 0.40 |
| $0.1 \times 10^{-10}$ | 0.137 | 0.349 |
| $1.0 \times 10^{-10}$ | 1.374 | 0.101 |
| $2.0 \times 10^{-10}$ | 2.748 | 0.026 |
| $5.0 \times 10^{-10}$ | 6.869 | 0.001 |
| $10.0 \times 10^{-10}$ | 13.74 | $\approx 0$ |

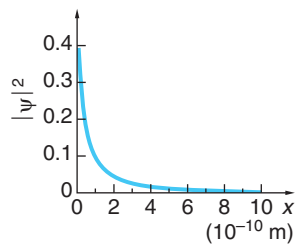



Figure 6-26

## Barrier Potential

Now let us consider one of the more interesting quantum-mechanical potentials, the barrier, illustrated by the example in Figure 6-27. The potential is

$$V(x) = \begin{cases} V_0 & \text{for} \quad 0 < x < a \\ 0 & \text{for} \quad 0 > x \quad \text{and} \quad x > a \end{cases} \qquad \textbf{6-73}$$

Classical particles incident on the barrier from the left in Region I with $E > V_0$ will all be transmitted, slowing down while passing through Region II but moving at their original speed again in Region III. For classical particles with $E < V_0$ incident from the left, all are reflected back into Region I. The quantum-mechanical behavior of particles incident on the barrier in both energy ranges is *much* different!

First, let us see what happens when a beam of particles, all with the same energy $E < V_0$, as illustrated in Figure 6-27*a*, are incident from the left. The general solutions to the wave equation are, following the example of the potential step,

$$\begin{aligned} \psi_I(x) &= Ae^{ik_1x} + Be^{-ik_1x} && x < 0 \\ \psi_{II}(x) &= Ce^{-\alpha x} + De^{\alpha x} && 0 < x < \alpha \\ \psi_{III}(x) &= Fe^{ik_1x} + Ge^{-ik_1x} && x > a \end{aligned} \qquad \textbf{6-74}$$

where, as before, $k_1 = \sqrt{2mE}/\hbar$ and $\alpha = \sqrt{2m(V_0 - E)}/\hbar$. Note that $\psi_{II}$ involves real exponentials, whereas $\psi_I$ and $\psi_{III}$ contain complex exponentials. Since the particle beam is incident on the barrier from the left, we can set $G = 0$. Once again, the value of $A$ is determined by the particle density in the beam and the four constants $B$, $C$, $D$, and $F$ are found in terms of $A$ by applying the continuity condition on $\psi$ and $d\psi/dx$ at $x = 0$ and at $x = a$. The details of the calculation are not of concern to us here, but several of the more interesting results are.

As we discovered for the potential step with $E < V_0$, the wave function incident from the left does not decrease immediately to zero at the barrier but instead will decay exponentially in the region of the barrier. Upon reaching the far wall of the barrier, the wave function must join smoothly to a sinusoidal wave function to the right of the barrier, as shown in Figure 6-27*b*. This implies that there will be some probability of the particles represented by the wave function being found on the far right side of the

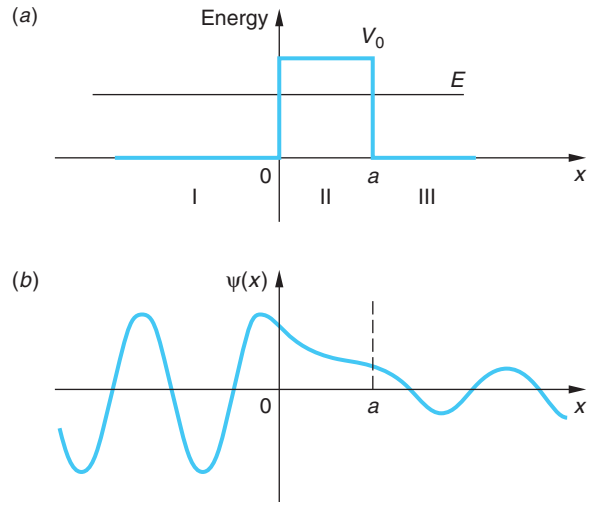



Figure 6-27 (*a*) Square barrier potential. (*b*) Penetration of the barrier by a wave with energy less than the barrier energy. Part of the wave is transmitted by the barrier even though, classically, the particle cannot enter the region $0 < x < a$ in which the potential energy is greater than the total energy.

barrier, although classically they should never be able to get through; i.e., there is a probability that the particles approaching the barrier can penetrate it. This phenomenon is called *barrier penetration* or *tunneling* (see Figure 6-28). The relative probability of its occurrence in any given situation is given by the transmission coefficient.

The coefficient of transmission $T$ from Region I into Region III is found to be (see Problem 6-64)

$$T = \frac{|F|^2}{|A|^2} = \left[1 + \frac{\sinh^2 \alpha a}{4\dfrac{E}{V_0}\left(1 - \dfrac{E}{V_0}\right)}\right]^{-1} \qquad \textbf{6-75}$$

If $\alpha a \gg 1$, Equation 6-75 takes on the somewhat simpler form to evaluate

$$T \approx 16\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)e^{-2\alpha a} \qquad \textbf{6-76}$$

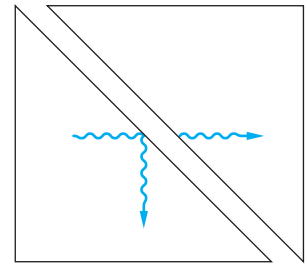


Figure 6-28 Optical barrier penetration, sometimes called frustrated total internal reflection. Because of the presence of the second prism, part of the wave penetrates the air barrier even though the angle of incidence in the first prism is greater than the critical angle. This effect can be demonstrated with two 45° prisms and a laser or a microwave beam and 45° prisms made of paraffin.

An important application of tunneling is the tunnel diode, a common component of electronic circuits. Another is *field emission*, tunneling of electrons facilitated by an electric field, now being used in wide-angle, flat-screen displays on some laptop computers.

*Scanning Tunneling Microscope* In the *scanning tunneling microscope* (STM), developed in the 1980s by G. Binnig and H. Rohrer, a narrow gap between a conducting specimen and the tip of a tiny probe acts as a potential barrier to electrons bound in the specimen, as illustrated in Figure 6-29. A small bias voltage applied between the probe and the specimen causes the electrons to tunnel through the barrier separating the two surfaces if the surfaces are close enough together. The tunneling current is extremely sensitive to the size of the gap, i.e., the width of the barrier, between the probe and specimen. A change of only 0.5 nm (about the diameter of one atom) in the width of the barrier can cause the tunneling current to change by as much as a factor of $10^4$. As the probe scans the specimen, a constant tunneling current is maintained by a piezoelectric feedback system that keeps the gap constant. Thus, the surface of the specimen can be mapped out by the vertical motions of the probe. In this way, the surface features of a specimen can be measured by STMs with a resolution of the order of the size of a single atom (see Figure 6-29).

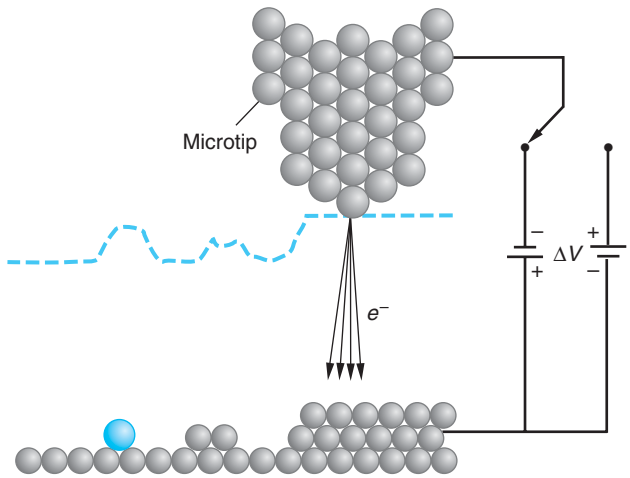
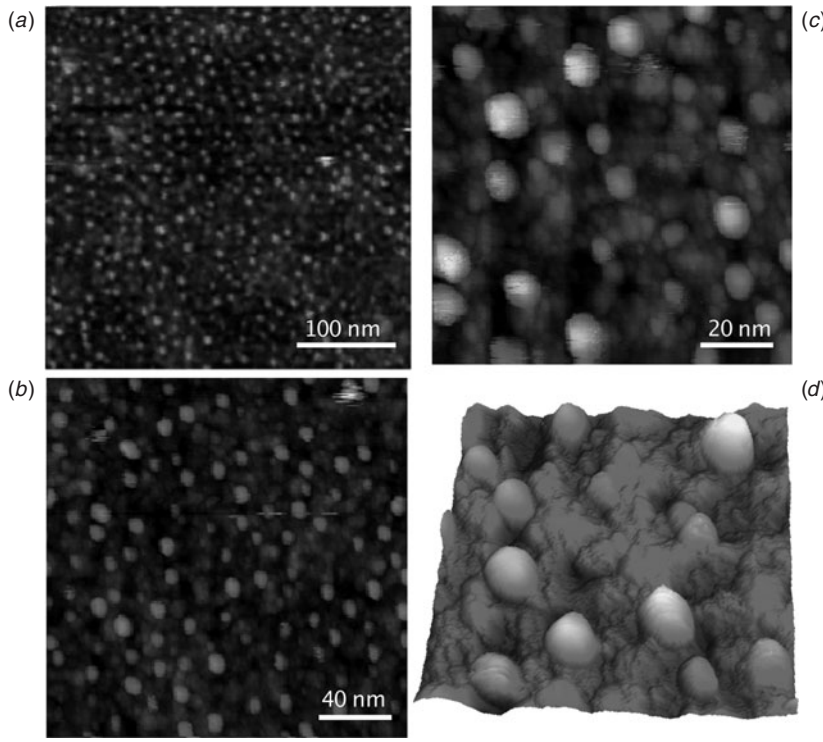



Figure 6-29 Schematic illustration of the path of the probe of an STM (dashed line) scanned across the surface of a sample while maintaining constant tunneling current. The probe has an extremely sharp microtip of atomic dimensions. Tunneling occurs over a small area across the narrow gap, allowing very small features (even individual atoms) to be imaged, as indicated by the dashed line.




Room temperature UHV-STM images of gold (Au) nanoparticles supported on TiC after annealing at 500°C. Images are (*a*) 375 nm × 375 nm, (*b*) 200 × 200 nm, and (*c*) 100 × 100 nm. (*d*) A 3-D image of a 70 nm × 70 nm section of (*c*). [*The authors thank Beatriz Roldán Cuenya for permission to use these STM images.*]

## EXPLORING
## Alpha Decay

Barrier penetration was used by G. Gamow, E. U. Condon, and R. W. Gurney in 1928 to explain the enormous variation in the mean life for α decay of radioactive nuclei and the seemingly paradoxical very existence of α decay.[16] While radioactive α decay will be discussed more thoroughly in Chapter 11, in general, the smaller the energy of the emitted α particle, the larger the mean life. The energies of α particles from natural radioactive sources range from about 4 to 7 MeV, whereas the mean lifetimes range from about $10^{10}$ years to $10^{-6}$ s. Gamow represented the radioactive nucleus by a potential well containing an α particle, as shown in Figure 6-30*a*. For $r$ less than the nuclear radius $R$, the α particle is attracted by the nuclear force. Without knowing much about this force, Gamow and his co-workers represented it by a square well. Outside the nucleus, the α particle is repelled by the Coulomb force. This is represented by the Coulomb potential energy $+kZze^2/r$, where $z = 2$ for the α particle and $Ze$ is the remaining nuclear charge. The energy $E$ is the measured kinetic energy of the emitted α particle, since when it is far from the nucleus its potential energy is zero. We see from the figure that a small increase in $E$ reduces the relative height of the barrier $V - E$ and also reduces the thickness. Because the probability of transmission varies exponentially with the relative height and barrier thickness, as indicated by Equation 6-76, a small increase in $E$ leads to a large increase in the probability of transmission and in turn to a shorter lifetime. Gamow and his co-workers were able to derive an expression for the α decay rate and the mean lifetime as a function of energy $E$ that was in good agreement with experimental results as follows:

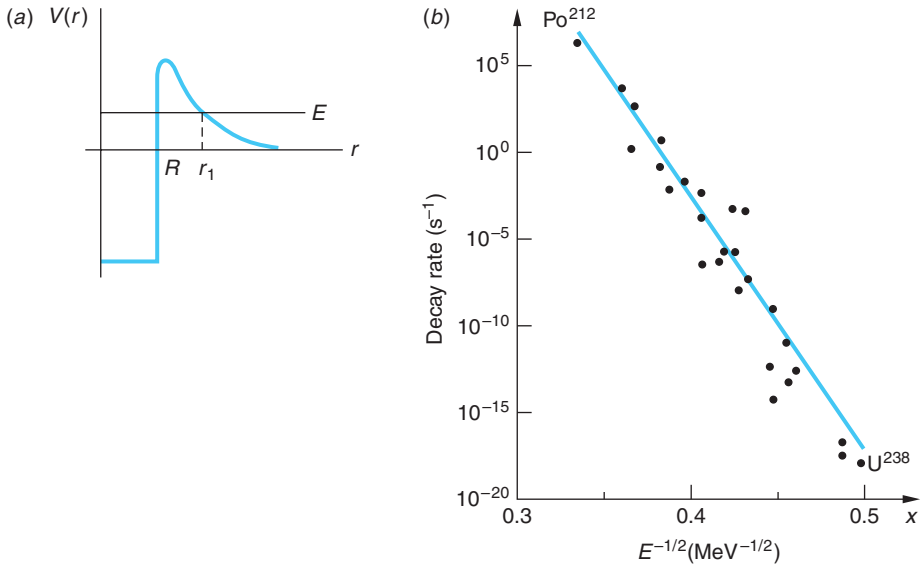



Figure 6-30 (*a*) Model of potential-energy function for an α particle and a nucleus. The strong attractive nuclear force for $r$ less than the nuclear radius $R$ can be approximately described by the potential well shown. Outside the nucleus the nuclear force is negligible, and the potential is given by Coulomb's law, $V(r) = +kZze^2/r$, where $Ze$ is the nuclear charge and $ze$ is the charge of the α particle. An α particle inside the nucleus oscillates back and forth, being reflected at the barrier at $R$. Because of its wave properties, when the α particle hits the barrier, there is a small chance that it will penetrate and appear outside the well at $r = r_1$. The wave function is similar to that shown in Figure 6-27*b*. (*b*) The decay rate for the emission of α particles from radioactive nuclei. The solid curve is the prediction of Equation 6-79; the points are experimental results.

The probability that an α particle will tunnel through the barrier in any one approach is given by $T$ from Equation 6-76. In fact, in this case $\alpha a$ is so large that the exponential dominates the expression and

$$T \approx e^{-2\sqrt{2m(V_0 - E)}a/\hbar} \qquad \textbf{6-77}$$

which is a very small number; i.e., the α particle is usually reflected. The number of times per second $N$ that the α particle approaches the barrier is given roughly by

$$N \approx \frac{v}{2R} \qquad \textbf{6-78}$$

where $v$ equals the particle's speed inside the nucleus. Thus, the decay rate, or the probability per second that the nucleus will emit an α particle, which is also the reciprocal of the mean life τ, is given by

$$\text{decay rate} = \frac{1}{\tau} = \frac{v}{2R} e^{-2\sqrt{2m(V_0 - E)}a/\hbar} \qquad \textbf{6-79}$$

Figure 6-30*b* illustrates the good agreement between the barrier penetration calculation and experimental measurements.

In the event that $E/V_0 > 1$, there is no reflected wave for $\alpha a = \pi, 2\pi, \ldots$ as a result of destructive interference. For electrons incident on noble gas atoms the resulting 100 percent transmission is called Ramsauer-Townsend effect and is a way of measuring atomic diameters for those elements.

## EXPLORING
## $NH_3$ Atomic Clock

Barrier penetration also takes place in the case of the periodic *inversion* of the ammonia molecule. The $NH_3$ molecule has two equilibrium configurations, as illustrated in Figure 6-31*a*. The three hydrogen atoms are arranged in a plane. The nitrogen atom oscillates between two equilibrium positions equidistant from each of the H atoms above and below the plane. The potential energy function $V(x)$ acting on the N atom has two minima located symmetrically about the center of the plane, as shown in Figure 6-31*b*. The N atom is bound to the molecule, so the energy is quantized and the lower states lie well below the central maximum of the potential. The central maximum presents a barrier to the N atoms in the lower states through which they slowly tunnel back and forth.[17] The oscillation frequency $f = 2.3786 \times 10^{10}$ Hz when the atom is in the state characterized by the energy $E_1$ in Figure 6-31*b*. This frequency is quite low compared with the frequencies of most molecular vibrations, a fact that allowed the N atom tunneling frequency in $NH_3$ to be used as the standard in the first *atomic clocks*, devices that now provide the world's standard for precision timekeeping.

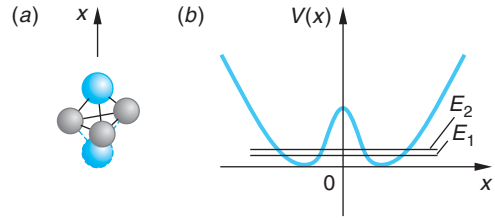



Figure 6-31 (*a*) The $NH_3$ molecule oscillates between the two equilibrium positions shown. The H atoms form a plane; the N atom is colored. (*b*) The potential energy of the N atom, where $x$ is the distance above and below the plane of the H atoms. Several of the allowed energies, including the two lowest shown, lie below the top of the central barrier through which the N atom tunnels.

## More

Quantum-mechanical tunneling involving two barriers is the basis for a number of devices such as the tunnel diode and the Josephson junction, both of which have a wide variety of useful applications. As an example of such systems, the *Tunnel Diode* is described on the home page: www.whfreeman.com/tiplermodernphysics5e. See also Equation 6-80 and Figure 6-32 here.

# Summary

| TOPIC | RELEVANT EQUATIONS AND REMARKS | |
|---|---|---|
| **1.** Schrödinger equation | | |
| Time dependent, one space dimension | $-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x,t)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}$ | **6-6** |