

# Chapter 6

## The Schrödinger Equation

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The success of the de Broglie relations in predicting the diffraction of electrons and other particles, and the realization that classical standing waves lead to a discrete set of frequencies, prompted a search for a wave theory of electrons analogous to the wave theory of light. In this electron wave theory, classical mechanics should appear as the short-wavelength limit, just as geometric optics is the short-wavelength limit of the wave theory of light. The genesis of the correct theory went something like this, according to Felix Bloch,<sup>1</sup> who was present at the time:

... in one of the next colloquia, Schrödinger gave a beautifully clear account of how de Broglie associated a wave with a particle and how he [i.e., de Broglie] could obtain the quantization rules ... by demanding that an integer number of waves should be fitted along a stationary orbit. When he had finished Debye<sup>2</sup> casually remarked that he thought this way of talking was rather childish ... [that to] deal properly with waves, one had to have a wave equation.

In 1926, Erwin Schrödinger<sup>3</sup> published his now-famous wave equation which governs the propagation of matter waves, including those of electrons. A few months earlier, Werner Heisenberg had published a seemingly different theory to explain atomic phenomena. In the Heisenberg theory, only measurable quantities appear. Dynamical quantities such as energy, position, and momentum are represented by matrices, the diagonal elements of which are the possible results of measurement. Though the Schrödinger and Heisenberg theories appear to be different, it was eventually shown by Schrödinger himself that they were equivalent, in that each could be derived from the other. The resulting theory, now called *wave mechanics* or *quantum mechanics*, has been amazingly successful. Though its principles may seem strange to us whose experiences are limited to the macroscopic world, although the mathematics required to solve even the simplest problem is quite involved, there seems to be no alternative to describe correctly the experimental results in atomic and nuclear physics. In this book we shall confine our study to the Schrödinger theory because it is easier to learn and is a little less abstract than the Heisenberg theory. We shall begin by restricting our discussion to problems in one space dimension.

## 6-1 The Schrödinger Equation in One Dimension

The wave equation governing the motion of electrons and other particles with mass, which is analogous to the classical wave equation (Equation 5-11), was found by Schrödinger late in 1925 and is now known as the *Schrödinger equation*. Like the classical wave equation, the Schrödinger equation relates the time and space derivatives of the wave function. The reasoning followed by Schrödinger is somewhat difficult and not important for our purposes. In any case, it must be emphasized that we can't derive the Schrödinger equation just as we can't derive Newton's laws of motion. Its validity, like that of any fundamental equation, lies in its agreement with experiment. Just as Newton's second law is not relativistically correct, neither is Schrödinger's equation, which must ultimately yield to a relativistic wave equation. But, as you know, Newton's laws of motion are perfectly satisfactory for solving a vast array of nonrelativistic problems. So, too, will be Schrödinger's equation when applied to the equally extensive range of nonrelativistic problems in atomic, molecular, and solid-state physics. Schrödinger tried without success to develop a relativistic wave equation, a task accomplished in 1928 by Dirac.

Although it would be logical merely to postulate the Schrödinger equation, we can get some idea of what to expect by first considering the wave equation for photons, which is Equation 5-11 with speed  $v = c$  and with  $y(x, t)$  replaced by the electric field  $\mathcal{E}(x, t)$ .

$$\frac{\partial^2 \mathcal{E}}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 \mathcal{E}}{\partial t^2} \quad 6-1$$

As discussed in Chapter 5, a particularly important solution of this equation is the harmonic wave function  $\mathcal{E}(x, t) = \mathcal{E}_0 \cos(kx - \omega t)$ . Differentiating this function twice, we obtain

$$\frac{\partial^2 \mathcal{E}}{\partial t^2} = -\omega^2 \mathcal{E}_0 \cos(kx - \omega t) = -\omega^2 \mathcal{E}(x, t)$$

and

$$\frac{\partial^2 \mathcal{E}}{\partial x^2} = -k^2 \mathcal{E}(x, t)$$

Substitution into Equation 6-1 then gives

$$-k^2 = -\frac{\omega^2}{c^2}$$

$$\omega = kc \quad 6-2$$

If  $\omega = E/\hbar$  and  $p = \hbar k$  for electromagnetic radiation, we have

$$E = pc \quad 6-3$$

which, as we saw earlier, is the relation between the energy and momentum of a photon.

Erwin Schrödinger. [Courtesy of the Niels Bohr Library, American Institute of Physics.]



Now let us use the de Broglie relations for a particle such as an electron to find the relation between  $\omega$  and  $k$  which is analogous to Equation 6-2 for photons. We can then use this relation to work backward and see how the wave equation for electrons must differ from Equation 6-1. The total energy (nonrelativistic) of a particle of mass  $m$  is

$$E = \frac{p^2}{2m} + V \quad 6-4$$

where  $V$  is the potential energy. Using the de Broglie relations, we obtain

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} + V \quad 6-5$$

This differs from Equation 6-2 for a photon because it contains the potential energy and because the angular frequency  $\omega$  does not vary linearly with  $k$ . Note that we get a factor of  $\omega$  when we differentiate a harmonic wave function with respect to time and a factor of  $k$  when we differentiate with respect to position. We expect, therefore, that the wave equation that applies to electrons will relate the *first* time derivative to the *second* space derivative, and will also involve the potential energy of the electron.

Finally, we require that the wave equation for electrons will be a differential equation that is linear in the wave function  $\Psi(x, t)$ . This ensures that, if  $\Psi_1(x, t)$  and  $\Psi_2(x, t)$  are both solutions of the wave equation for the same potential energy, any arbitrary linear combination of these solutions is also a solution—i.e.,  $\Psi(x, t) = a_1\Psi_1(x, t) + a_2\Psi_2(x, t)$  is a solution, with  $a_1$  and  $a_2$  being arbitrary constants. Such a combination is called *linear* because both  $\Psi_1(x, t)$  and  $\Psi_2(x, t)$  appear only to the first power. Linearity guarantees that the wave functions will add together to produce constructive and destructive interference, which we have seen to be a characteristic

of matter waves, as well as all other wave phenomena. Note, in particular, that (1) the linearity requirement means that *every* term in the wave equation must be linear in  $\Psi(x, t)$  and (2) that *any* derivative of  $\Psi(x, t)$  is linear in  $\Psi(x, t)$ .<sup>4</sup>

### The Schrödinger Equation

We are now ready to postulate the Schrödinger equation for a particle of mass  $m$ . In one dimension, it has the form

$$\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2} + V(x, t) \Psi(x, t) = i\hbar \frac{\partial \Psi(x, t)}{\partial t} \quad 6-6$$

We will now show that this equation is satisfied by a harmonic wave function in the special case of a free particle, one on which no net force acts, so that the potential energy is constant,  $V(x, t) = V_0$ . First note that a function of the form  $\cos(kx - \omega t)$  does not satisfy this equation because differentiation with respect to time changes the cosine to a sine, but the second derivative with respect to  $x$  gives back a cosine. Similar reasoning rules out the form  $\sin(kx - \omega t)$ . However, the exponential form of the harmonic wave function does satisfy the equation. Let

$$\begin{aligned} \Psi(x, t) &= Ae^{i(kx - \omega t)} \\ &= A[\cos(kx - \omega t) + i \sin(kx - \omega t)] \end{aligned} \quad 6-7$$

where  $A$  is a constant. Then

$$\frac{\partial \Psi}{\partial t} = -i\omega Ae^{i(kx - \omega t)} = -i\omega \Psi$$

$$\frac{\partial^2 \Psi}{\partial x^2} = (ik^2) Ae^{i(kx - \omega t)} = -k^2 \Psi$$

Substituting these derivatives into the Schrödinger equation with  $V(x, t) = V_0$  gives

$$\frac{-\hbar^2}{2m} (-k^2 \Psi) + V_0 \Psi = i\hbar (-i\omega) \Psi$$

$$\frac{\hbar^2 k^2}{2m} + V_0 = \hbar \omega$$

which is Equation 6-5.

An important difference between the Schrödinger equation and the classical wave equation is the explicit appearance<sup>5</sup> of the imaginary number  $i = (-1)^{1/2}$ . The wave functions that satisfy the Schrödinger equation are not necessarily real, as we saw from the case of the free-particle wave function of Equation 6-7. Evidently the wave function  $\Psi(x, t)$  which solves the Schrödinger equation is not a directly

measurable function like the classical wave function  $y(x, t)$ , since measurements always yield real numbers. However, as we discussed in Section 5-4, the probability of finding the electron in  $dx$  is certainly measurable, just as is the probability that a flipped coin will turn up heads. The probability  $P(x) dx$  that the electron will be found in the volume  $dx$  was defined by Equation 5-26 to be equal to  $\Psi^2 dx$ . This probabilistic interpretation of  $\Psi$  was developed by Max Born and was recognized, over the early and formidable objections of both Schrödinger and Einstein, as the appropriate way of relating solutions of the Schrödinger equation to the results of physical measurements. The probability that an electron is in the region  $dx$ , a real number, can be measured by counting the fraction of time it is found there in a very large number of identical trials. In recognition of the complex nature of  $\Psi(x, t)$ , we must modify slightly the interpretation of the wave function discussed in Chapter 5 to accommodate Born's interpretation so that the probability of finding the electron in  $dx$  is real. We take for the probability

$$P(x, t) dx = \Psi^*(x, t) \Psi(x, t) dx = |\Psi(x, t)|^2 dx \quad 6-8$$

where  $\Psi^*$ , the complex conjugate of  $\Psi$ , is obtained from  $\Psi$  by replacing  $i$  with  $-i$  wherever it appears.<sup>6</sup> The complex nature of  $\Psi$  serves to emphasize the fact that we should not ask or try to answer the question, "What is waving in a matter wave?" or inquire as to what medium supports the motion of a matter wave. The wave function is a computational device with utility in Schrödinger's theory of wave mechanics. Physical significance is associated not with  $\Psi$  itself, but with the product  $\Psi^*\Psi = |\Psi|^2$ , which is the probability distribution  $P(x, t)$  or, as it is often called, the *probability density*. In keeping with the analogy with classical waves and wave functions  $\Psi(x, t)$  is also sometimes referred to as the *probability density amplitude*, or just the *probability amplitude*.

The probability of finding the electron in  $dx$  at  $x_1$  or in  $dx$  at  $x_2$  is the sum of separate probabilities,  $P(x_1) dx + P(x_2) dx$ . Since the electron must certainly be somewhere in space, the sum of the probabilities over all possible values of  $x$  must equal 1. That is,<sup>7</sup>

$$\int_{-\infty}^{+\infty} \Psi^*\Psi dx = 1 \quad 6-9$$

Equation 6-9 is called the *normalization condition*. This condition plays an important role in quantum mechanics, for it places a restriction on the possible solutions of the Schrödinger equation. In particular, the wave function  $\Psi(x, t)$  must approach zero sufficiently fast as  $x \rightarrow \pm\infty$  so that the integral in Equation 6-9 remains finite. If it does not, then the probability becomes unbounded. As we will see in Section 6-3, this restriction together with boundary conditions imposed at finite values of  $x$  then leads to energy quantization for bound particles.

In the chapters that follow we are going to be concerned with solutions to the Schrödinger equation for a wide range of real physical systems, but in what follows in this chapter our intent is to illustrate a few of the techniques of solving the equation and to discover the various, often surprising properties of the solutions. To the end we will focus our attention on one-dimensional problems, as noted earlier, and use some potential energy functions with unrealistic physical characteristics, e.g., infinitely rigid walls, which will enable us to illustrate various properties of the solutions without obscuring the discussion with overly complex mathematics.

### Separation of the Time and Space Dependencies of $\Psi(x, t)$

Schrödinger's first application of his wave equation was to problems such as the hydrogen atom (Bohr's work) and the simple harmonic oscillator (Planck's work), in which he showed that the energy quantization in those systems can be explained naturally in terms of standing waves. We referred to these in Chapter 4 as stationary states, meaning they did not change with time. Such states are also called *eigenstates*. For such problems that also have potential energy functions that are independent of time, the space and time dependence of the wave function can be separated, leading to a greatly simplified form of the Schrödinger equation.<sup>8</sup> The separation is accomplished by first assuming that  $\Psi(x, t)$  can be written as a product of two functions, one of  $x$  and one of  $t$ , as

$$\Psi(x, t) = \psi(x) \phi(t) \quad 6-10$$

If Equation 6-10 turns out to be incorrect, we will find that out soon enough, but if the potential function is *not* an explicit function of time, i.e., if the potential is given by  $V(x)$ , our assumption turns out to be valid. That this is true can be seen as follows:

Substituting  $\Psi(x, t)$  from Equation 6-10 into the general, time-dependent Schrödinger equation (Equation 6-6) yields

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \psi(x) \phi(t)}{\partial x^2} + V(x) \psi(x) \phi(t) = i\hbar \frac{\partial \psi(x) \phi(t)}{\partial t} \quad 6-11$$

which is

$$\frac{-\hbar^2}{2m} \phi(t) \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x) \phi(t) = i\hbar \psi(x) \frac{d\phi(t)}{dt} \quad 6-12$$

where the derivatives are now ordinary rather than partial ones. Dividing Equation 6-12 by  $\Psi$  in the assumed product form  $\psi \phi$  gives

$$\frac{-\hbar^2}{2m} \frac{1}{\psi(x)} \frac{d^2 \psi(x)}{dx^2} + V(x) = i\hbar \frac{1}{\phi(t)} \frac{d\phi(t)}{dt} \quad 6-13$$

Notice that each side of Equation 6-13 is a function of only one of the independent variables  $x$  and  $t$ . This means that, for example, changes in  $t$  cannot affect the value of the left side of Equation 6-13, and changes in  $x$  cannot affect the right side. Thus, both sides of the equation must be equal to the same constant  $C$ , called the *separation constant*, and we see that the assumption of Equation 6-10 is valid—the variables have been separated. We have thus replaced a partial differential equation containing two independent variables, Equation 6-6, with two ordinary differential equations, each a function of only one of the independent variables:

$$\frac{-\hbar^2}{2m} \frac{1}{\psi(x)} \frac{d^2 \psi(x)}{dx^2} + V(x) = C \quad 6-14$$

$$i\hbar \frac{1}{\phi(t)} \frac{d\phi(t)}{dt} = C \quad 6-15$$

Let us solve Equation 6-15 first. The reason for doing so is twofold: (1) Equation 6-15 does not contain the potential  $V(x)$ ; consequently, the time-dependent part  $\phi(t)$

of all solutions  $\Psi(x, t)$  to the Schrödinger equation will have the same form when the potential is not an explicit function of time, so we only have to do this once. (2) The separation constant  $C$  has particular significance that we want to discover before we tackle Equation 6-14. Writing Equation 6-15 as

$$\frac{d\phi(t)}{\phi(t)} = \frac{C}{i\hbar} dt = -\frac{iC}{\hbar} dt \quad 6-16$$

The general solution of Equation 6-16 is

$$\phi(t) = e^{-iCt/\hbar} \quad 6-17a$$

which can also be written as

$$\phi(t) = e^{-iCt/\hbar} = \cos\left(\frac{Ct}{\hbar}\right) - i \sin\left(\frac{Ct}{\hbar}\right) = \cos\left(2\pi\frac{Ct}{h}\right) - i \sin\left(2\pi\frac{Ct}{h}\right) \quad 6-17b$$

Thus we see that  $\phi(t)$ , which describes the time variation of  $\Psi(x, t)$ , is an oscillatory function with frequency  $f = C/h$ . However, according to the de Broglie relation (Equation 5-1), the frequency of the wave represented by  $\Psi(x, t)$  is  $f = E/h$ ; therefore, we conclude that the separation constant  $C = E$ , the total energy of the particle, and we have

$$\phi(t) = e^{-iEt/\hbar} \quad 6-17c$$

for all solutions to Equation 6-6 involving time-independent potentials. Equation 6-14 then becomes, on multiplication by  $\psi(x)$ ,

$$\frac{-\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \quad 6-18$$

Equation 6-18 is referred to as the *time-independent Schrödinger equation*.

The time-independent Schrödinger equation in one dimension is an ordinary differential equation in one variable  $x$  and is therefore much easier to handle than the general form of Equation 6-6. The normalization condition of Equation 6-9 can be expressed in terms of  $\psi(x)$ , since the time dependence of the absolute square of the wave function cancels. We have

$$\Psi^*(x, t)\Psi(x, t) = \psi^*(x)e^{+iEt/\hbar}\psi(x)e^{-iEt/\hbar} = \psi^*(x)\psi(x) \quad 6-19$$

and Equation 6-9 then becomes

$$\int_{-\infty}^{+\infty} \psi^*(x)\psi(x)dx = 1 \quad 6-20$$

### Conditions for Acceptable Wave Functions

The form of the wave function  $\psi(x)$  that satisfies Equation 6-18 depends on the form of the potential energy function  $V(x)$ . In the next few sections we shall study

simple but important problems in which  $V(x)$  is specified. Our example potentials will be approximations to real physical potentials, simplified to make calculations easier. In some cases, the slope of the potential energy may be discontinuous, e.g.,  $V(x)$  may have one form in one region of space and another form in an adjacent region. (This is a useful mathematical approximation to real situations in which  $V(x)$  varies rapidly over a small region of space, such as at the surface boundary of a metal.) The procedure in such cases is to solve the Schrödinger equation separately in each region of space, and then require that the solutions join smoothly at the point of discontinuity.

Since the probability of finding a particle cannot vary discontinuously from point to point, the wave function  $\psi(x)$  must be continuous.<sup>9</sup> Since the Schrödinger equation involves the second derivative  $d^2\psi/d^2x = \psi''(x)$ , the first derivative  $\psi'$  (which is the slope) must also be continuous. That is, the graph of  $\psi(x)$  versus  $x$  must be smooth. (In a special case in which the potential energy becomes infinite, this restriction is relaxed. Since no particle can have infinite potential energy,  $\psi(x)$  must be zero in regions where  $V(x)$  is infinite. Then, at the boundary of such a region,  $\psi'$  may be discontinuous.)

If either  $\psi(x)$  or  $d\psi/dx$  were not finite or not single-valued, the same would be true of  $\Psi(x, t)$  and  $d\Psi/dx$ . As we will shortly see, the predictions of wave mechanics regarding the results of measurements involve both of those quantities and would thus not necessarily predict finite or definite values for real physical quantities. Such results would not be acceptable, since measurable quantities, such as angular momentum and position, are never infinite or multiple-valued. A final restriction on the form of the wave function  $\psi(x)$  is that in order to obey the normalization condition,  $\psi(x)$  must approach zero sufficiently fast as  $x \rightarrow \pm\infty$  so that normalization is preserved. For future reference, we may summarize the conditions that the wave function  $\psi(x)$  must meet in order to be acceptable as follows:

1.  $\psi(x)$  must exist and satisfy the Schrödinger equation.
2.  $\psi(x)$  and  $d\psi/dx$  must be continuous.
3.  $\psi(x)$  and  $d\psi/dx$  must be finite.
4.  $\psi(x)$  and  $d\psi/dx$  must be single-valued.
5.  $\psi(x) \rightarrow 0$  fast enough as  $x \rightarrow \pm\infty$  so that the normalization integral, Equation 6-20, remains bounded.

#### QUESTIONS

Like the classical wave equation, the Schrödinger equation is linear. Why is this important?

There is no factor  $i = (-1)^{1/2}$  in Equation 6-18. Does this mean that  $\psi(x)$  must be real?

Why must the electric field  $\mathcal{E}(x, t)$  be real? Is it possible to find a nonreal wave function that satisfies the classical wave equation?

Describe how the de Broglie hypothesis enters into the Schrödinger wave equation.

What would be the effect on the Schrödinger equation of adding a constant rest energy for a particle with mass to the total energy  $E$  in the de Broglie relation  $f = E/h$ ?

Describe in words what is meant by normalization of the wave function.



**EXAMPLE 6-1 A Solution to the Schrödinger Equation** Show that for a free particle of mass  $m$  moving in one dimension the function  $\psi(x) = A \sin kx + B \cos kx$  is a solution to the time-independent Schrödinger equation for any values of the constants  $A$  and  $B$ .

**Solution**

A free particle has no net force acting upon it, e.g.,  $V(x) = 0$ , in which case the kinetic energy equals the total energy. Thus,  $p = \hbar k = (2mE)^{1/2}$ . Differentiating  $\psi(x)$  gives

$$\frac{d\psi}{dx} = kA \cos kx - kB \sin kx$$

and differentiating again,

$$\begin{aligned} \frac{d^2\psi}{dx^2} &= -k^2A \sin kx - k^2B \cos kx \\ &= -k^2(A \sin kx + B \cos kx) = -k^2\psi(x) \end{aligned}$$

Substituting into Equation 6-18,

$$\begin{aligned} \frac{-\hbar^2}{2m} [(-k^2)(A \sin kx + B \cos kx)] &= E[A \sin kx + B \cos kx] \\ \frac{\hbar^2 k^2}{2m} \psi(x) &= E\psi(x) \end{aligned}$$

and, since  $\hbar^2 k^2 = 2mE$ , we have

$$E\psi(x) = E\psi(x)$$

and the given  $\psi(x)$  is a solution of Equation 6-18.

## 6-2 The Infinite Square Well

A problem that provides several illustrations of the properties of wave functions and also one of the easiest problems to solve using the time-independent, one-dimensional Schrödinger equation is that of the infinite square well, sometimes called the particle in a box. A macroscopic example is a bead moving on a frictionless wire between two massive stops clamped to the wire. We could also build such a "box" for an electron using electrodes and grids in an evacuated tube as illustrated in Figure 6-1a. The walls of the box are provided by the increasing potential between the grids  $G$  and the electrode  $C$  as shown in Figures 6-1b and c. The walls can be made arbitrarily high and steep by increasing the potential  $V$  and reducing the separation between each electrode pair. In the limit such a potential energy function looks like that shown

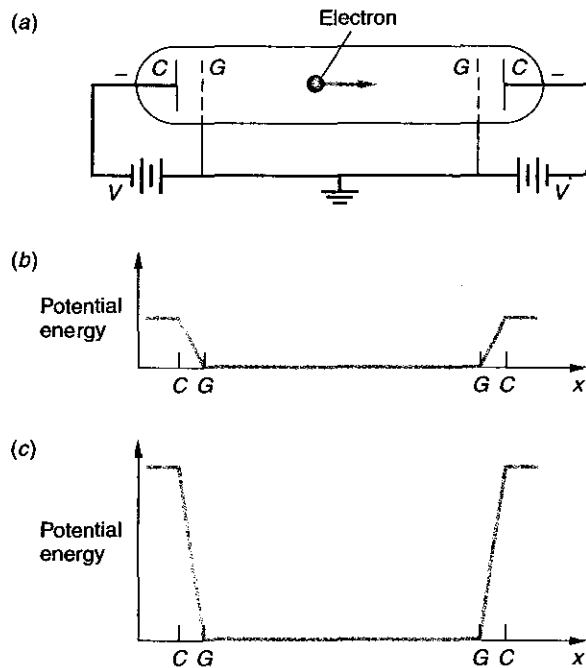


Fig. 6-1 (a) The electron placed between the two sets of electrodes  $C$  and grids  $G$  experiences no force in the region between the grids, which are at ground potential. However, in the regions between each  $C$  and  $G$  is a repelling electric field whose strength depends upon the magnitude of  $V$ . (b) If  $V$  is small, then the electron's potential energy vs.  $x$  has low, sloping "walls." (c) If  $V$  is large, the "walls" become very high and steep, becoming infinitely high for  $V \rightarrow \infty$ .

Figure 6-2, which is a graph of the potential energy of an infinite square well. For this problem the potential energy is of the form

$$\begin{aligned} V(x) &= 0 & 0 < x < L \\ V(x) &= \infty & x < 0 \text{ and } x > L \end{aligned} \quad 6-21$$

Although such a potential is clearly artificial, the problem is worth careful study for several reasons: (1) exact solutions to the Schrödinger equation can be obtained without the difficult mathematics which usually accompanies its solution for more realistic potential functions; (2) the problem is closely related to the vibrating-string problem familiar in classical physics; (3) it illustrates many of the important features of all quantum-mechanical problems; and finally (4) this potential is a relatively good approximation to some real situations; e.g., the motion of a free electron inside a metal.

Since the potential energy is infinite outside the well, the wave function is required to be zero there; that is, the particle must be inside the well. (As we proceed through this and other problems, keep in mind Born's interpretation: the probability density of the particle's position is proportional to  $|\psi|^2$ .) We then need only to solve Equation 6-18 for the region inside the well  $0 < x < L$ , subject to the condition that since the wave function must be continuous,  $\psi(x)$  must be zero at  $x = 0$  and  $x = L$ . Each condition on the wave function at a boundary (here, the discontinuity of the potential energy function) is called a *boundary condition*. We shall see that, mathematically, it is the boundary conditions together with the requirement that  $\psi(x) \rightarrow 0$  as  $x \rightarrow \pm\infty$  that lead to the quantization of energy. A classic example is the case of a vibrating string fixed at both ends. In that case the wave function  $y(x, t)$  is the displacement of the string. If the string is fixed at  $x = 0$  and  $x = L$ , we have the same boundary condition on the vibrating-string wave function: namely, that  $y(x, t)$  be zero at  $x = 0$  and  $x = L$ . These boundary conditions lead to discrete allowed frequencies

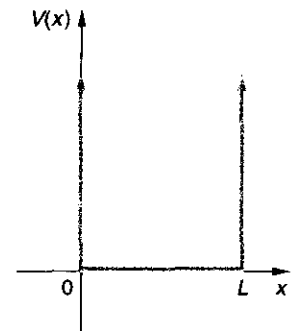


Fig. 6-2 Infinite square well potential energy. For  $0 < x < L$  the potential energy  $V(x)$  is zero. Outside this region,  $V(x)$  is infinite. The particle is confined to the region in the well  $0 < x < L$ .

of vibration of the string. It was this quantization of frequencies (which always occurs for standing waves in classical physics), along with de Broglie's hypothesis, which motivated Schrödinger to look for a wave equation for electrons.

The standing-wave condition for waves on a string of length  $L$  fixed at both ends is that *an integral number of half wavelengths fit into the length  $L$ .*

$$n \frac{\lambda}{2} = L \quad n = 1, 2, 3, \dots \quad 6-22$$

We shall show below that the same condition follows from the solution of the Schrödinger equation for a particle in an infinite square well. Since the wavelength is related to the momentum of the particle by the de Broglie relation  $p = h/\lambda$  and the total energy of the particle in the well is just the kinetic energy  $p^2/2m$  (see Figure 6-1), this quantum condition on the wavelength implies that the energy is quantized and the allowed values are given by

$$E = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{h^2}{2m(2L/n)^2} = n^2 \frac{h^2}{8mL^2} \quad 6-23$$

Since the energy depends on the integer  $n$ , it is customary to label it  $E_n$ . In terms of  $\hbar = h/2\pi$  the energy is given by

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} = n^2 E_1 \quad n = 1, 2, 3, \dots \quad 6-24$$

where  $E_1$  is the lowest allowed energy<sup>10</sup> and is given by

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2} \quad 6-25$$

We now derive this result from the time-independent Schrödinger equation (Equation 6-18), which for  $V(x) = 0$  is

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

or 
$$\psi''(x) = -\frac{2mE}{\hbar^2} \psi(x) = -k^2\psi(x) \quad 6-26$$

where we have substituted the square of the wave number  $k$ , since

$$k^2 = \left(\frac{p}{\hbar}\right)^2 = \frac{2mE}{\hbar^2} \quad 6-27$$

and have written  $\psi''(x)$  for the second derivative  $d^2\psi(x)/dx^2$ . Equation 6-26 has solutions of the form

$$\psi(x) = A \sin kx \quad 6-28$$

and 
$$\psi(x) = B \cos kx \quad 6-28$$

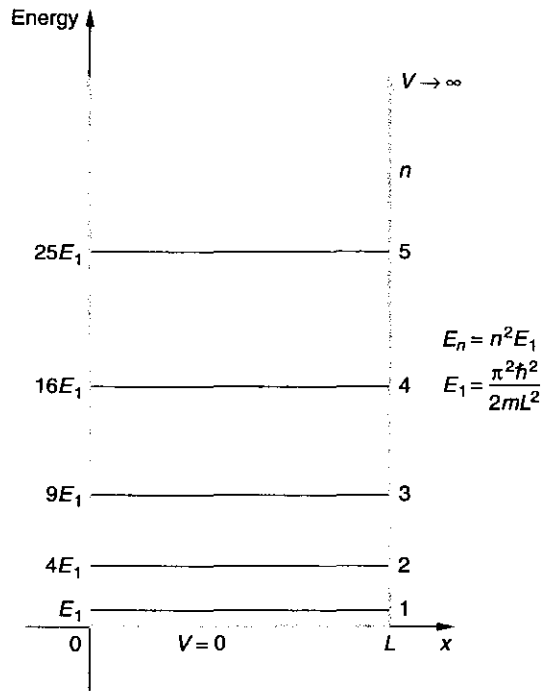


Fig. 6-3 Graph of energy vs.  $x$  for a particle in an infinitely deep well. The potential energy  $V(x)$  is shown with the colored lines. The set of allowed values for the particle's total energy  $E_n$  as given by Equation 6-24 form the energy-level diagram for the infinite square well potential. Classically, a particle can have any value of energy. Quantum mechanically, only the values given by  $E_n = n^2(\hbar^2\pi^2/2mL^2)$  yield well-behaved solutions of the Schrödinger equation. As we become more familiar with energy-level diagrams, the  $x$  axis will be omitted.

where  $A$  and  $B$  are constants. The boundary condition  $\psi(x) = 0$  at  $x = 0$  rules out the cosine solution (Equation 6-28b) because  $\cos 0 = 1$ , so  $B$  must equal zero. The boundary condition  $\psi(x) = 0$  at  $x = L$  gives

$$\psi(L) = A \sin kL = 0 \tag{6-29}$$

This condition is satisfied if  $kL$  is any integer times  $\pi$ , i.e., if  $k$  is restricted to the values  $k_n$  given by

$$k_n = n \frac{\pi}{L} \quad n = 1, 2, 3, \dots \tag{6-30}$$

If we write the wave number  $k$  in terms of the wavelength  $\lambda = 2\pi/k$ , we see that Equation 6-30 is the same as Equation 6-22 for standing waves on a string. The quantized energy values, or *energy eigenvalues*, are found from Equation 6-27, replacing  $k$  by  $k_n$  as given by Equation 6-30. We thus have

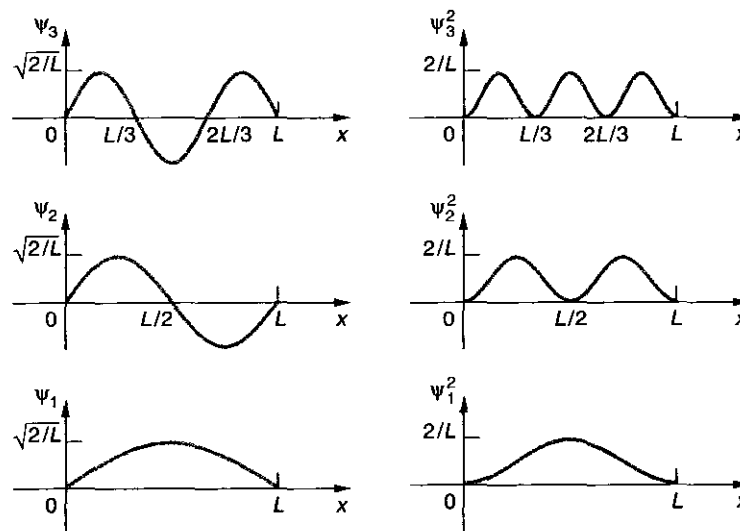
$$E_n = \frac{\hbar^2 k_n^2}{2m} = n^2 \frac{\hbar^2 \pi^2}{2mL^2} = n^2 E_1$$

which is the same as Equation 6-24. Figure 6-3 shows the energy-level diagram and the potential energy function for the infinite square well potential.

The constant  $A$  in the wave function of Equation 6-28a is determined by the normalization condition

$$\int_{-\infty}^{+\infty} \psi_n^* \psi_n dx = \int_0^L A_n^2 \sin^2 \left( \frac{n\pi x}{L} \right) dx = 1 \tag{6-31}$$

**Fig. 6-4** Wave functions  $\psi_n(x)$  and probability densities  $P_n(x) = \psi_n^2(x)$  for  $n = 1, 2,$  and  $3$  for the infinite square well potential.



Since the wave function is zero in regions of space where the potential energy is infinite, the contributions to the integral from  $-\infty$  to  $0$  and from  $L$  to  $+\infty$  will both be zero. Thus, only the integral from  $0$  to  $L$  needs to be evaluated. Integrating, we obtain  $A_n = (2/L)^{1/2}$ , independent of  $n$ , a result first encountered in the solution to Problem 5-24. The normalized wave function solutions for this problem, also called *eigenfunctions*, are then

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad n = 1, 2, 3, \dots \quad 6-32$$

These wave functions are exactly the same as the standing-wave functions  $y_n(x)$  for the vibrating-string problem. The wave functions and the probability distribution functions  $P_n(x)$  are sketched in Figure 6-4 for the lowest energy state  $n = 1$ , called the *ground state*, and for the first two *excited states*,  $n = 2$  and  $n = 3$ . (Since these wave functions are real,  $P_n(x) = \psi_n^* \psi_n = \psi_n^2$ .) Notice in Figure 6-4 that the maximum amplitudes of each of the  $\psi_n(x)$  are the same,  $(2/L)^{1/2}$ , as are those of  $P_n(x)$ ,  $2/L$ . Note, too, that both  $\psi_n(x)$  and  $P_n(x)$  extend to  $\pm\infty$ . They just happen to be zero for  $x < 0$  and  $x > L$  in this case.

The number  $n$  in the equations above is called a *quantum number*. It specifies both the energy and the wave function. Given any value of  $n$  we can immediately write down the wave function and the energy of the system. The quantum number occurs because of the boundary conditions  $\psi(x) = 0$  at  $x = 0$  and  $x = L$ . We shall see in Section 7-1 that for problems in three dimensions, three quantum numbers arise, one associated with boundary conditions on each coordinate.

### Comparison with Classical Results

Let us compare our quantum-mechanical solution of this problem with the classical solution. In classical mechanics, if we know the potential energy function  $V(x)$ , we can find the force from  $F_x = -dV/dx$ , and thereby obtain the acceleration  $a_x = d^2x/dt^2$  from Newton's second law. We can then find the position  $x$  as a function of time  $t$  if we know the initial position and velocity. In this problem there is no fo

when the particle is between the walls of the well because  $V = 0$  there. The particle therefore moves with constant speed in the well. Near the edge of the well the potential energy rises discontinuously to infinity—we may describe this as a very large force that acts over a very short distance and turns the particle around at the wall so that it moves away with its initial speed. Any speed, and therefore any energy, is permitted classically. The classical description breaks down because, according to the uncertainty principle, we can never precisely specify both the position and momentum (and therefore velocity) at the same time. We can therefore never specify the initial conditions precisely, and cannot assign a definite position and momentum to the particle. Of course, for a macroscopic particle moving in a macroscopic box, the energy is much larger than  $E_1$  of Equation 6-25, and the minimum uncertainty of momentum, which is of the order of  $\hbar/L$ , is much less than the momentum and less than experimental uncertainties. Then the difference in energy between adjacent states will be a small fraction of the total energy, quantization will be unnoticed, and the classical description will be adequate.<sup>11</sup>

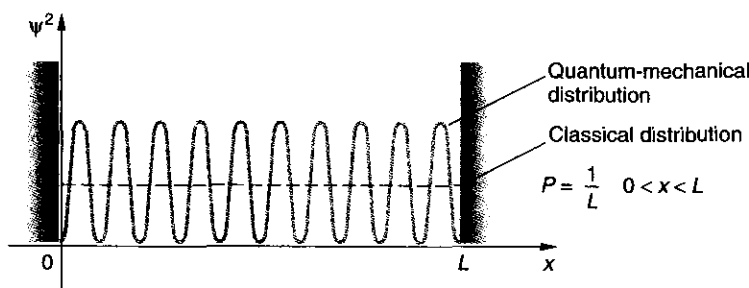
Let us also compare the classical prediction for the distribution of measurements of position with those from our quantum-mechanical solution. Classically, the probability of finding the particle in some region  $dx$  is proportional to the time spent in  $dx$ , which is  $dx/v$ , where  $v$  is the speed. Since the speed is constant, the classical distribution function is just a constant inside the well. The normalized classical distribution function is

$$P_C(x) = \frac{1}{L}$$

In Figure 6-4 we see that for the lowest energy states the quantum distribution function is very different from this. According to Bohr's correspondence principle, the quantum distributions should approach the classical distribution when  $n$  is large, that is, large energies. For any state  $n$ , the quantum distribution has  $n$  peaks. The distribution for  $n = 10$  is shown in Figure 6-5. For very large  $n$ , the peaks are close together, and if there are many peaks in a small distance  $\Delta x$  only the average value will be observed. The average value of  $\sin^2 k_n x$  over one or more cycles is  $1/2$ . Thus

$$[\psi_n^2(x)]_{\text{av}} = \left[ \frac{2}{L} \sin^2 k_n x \right]_{\text{av}} = \frac{2}{L} \frac{1}{2} = \frac{1}{L}$$

which is the same as the classical distribution.



6-5 Probability distribution for  $n = 10$  for the infinite square well potential. The dashed line is the classical probability density  $P = 1/L$ , which is equal to the quantum-mechanical distribution averaged over a region  $\Delta x$  containing several oscillations. A physical measurement with resolution  $\Delta x$  will yield the classical result if  $n$  is so large that  $\psi^2(x)$  has many oscillations in  $\Delta x$ .

### The Complete Wave Function

The complete wave function, including its time dependence, is found by multiplying the space part by

$$e^{-i\omega t} = e^{-i(E_n/\hbar)t}$$

according to Equation 6-17. As mentioned previously, a wave function corresponding to a single energy oscillates with angular frequency,  $\omega_n = E_n/\hbar$ , but the probability distribution  $|\Psi_n(x, t)|^2$  is independent of time. This is the wave-mechanical justification for calling such a state a stationary state or eigenstate, as we have done earlier. It is instructive to look at the complete wave function for a particular state  $n$ :

$$\Psi_n(x, t) = \sqrt{\frac{2}{L}} \sin k_n x e^{-i\omega_n t}$$

If we use the identity

$$\sin k_n x = \frac{(e^{ik_n x} - e^{-ik_n x})}{2i}$$

we can write this wave function as

$$\Psi_n(x, t) = \frac{1}{2i} \sqrt{\frac{2}{L}} [e^{i(k_n x - \omega_n t)} - e^{-i(k_n x + \omega_n t)}]$$

Just as in the case of the standing-wave function for the vibrating string, we can consider this stationary-state wave function to be the superimposition of a wave traveling to the right and a wave of the same frequency and amplitude traveling to the left.

**EXAMPLE 6-2** An Electron in a Wire An electron moving in a thin metal wire is a reasonable approximation of a particle in a one-dimensional infinite well. The potential inside the wire is constant on the average, but rises sharply at each end. Suppose the electron is in a wire 1.0 cm long. (a) Compute the ground-state energy for the electron. (b) If the electron's energy is equal to the average kinetic energy of the molecules in a gas at  $T = 300$  K, about 0.03 eV, what is the electron's quantum number  $n$ ?

#### Solution

- For question (a), the ground-state energy is given by Equation 6-25:

$$\begin{aligned} E_1 &= \frac{\pi^2 \hbar^2}{2mL^2} \\ &= \frac{\pi^2 (1.055 \times 10^{-34} \text{ J}\cdot\text{s})^2}{(2)(9.11 \times 10^{-31} \text{ kg})(10^{-2} \text{ m})^2} \\ &= 6.03 \times 10^{-34} \text{ J} = 3.80 \times 10^{-15} \text{ eV} \end{aligned}$$

2. For question (b), the electron's quantum number is given by Equation 6-24:

$$E_n = n^2 E_1$$

3. Solving Equation 6-24 for  $n$  and substituting  $E_n = 0.03 \text{ eV}$  and  $E_1$  from above yield:

$$n^2 = \frac{E_n}{E_1}$$

or

$$\begin{aligned} n &= \sqrt{\frac{E_n}{E_1}} \\ &= \sqrt{\frac{0.03 \text{ eV}}{3.80 \times 10^{-15} \text{ eV}}} \\ &= 2.81 \times 10^6 \end{aligned}$$

*Remarks:* The value of  $E_1$  computed above is not only far below the limit of measurability, but also smaller than the uncertainty in the energy of an electron confined into 1 cm.

**EXAMPLE 6-3** Calculating Probabilities Suppose that the electron in Example 6-2 could be measured while in its ground state. (a) What would be the probability of finding it somewhere in the region  $0 < x < L/4$ ? (b) What would be the probability of finding it in a very narrow region  $\Delta x = 0.01L$  wide centered at  $x = 5L/8$ ?

**Solution**

(a) The wave function for the  $n = 1$  level, the ground state, is given by Equation 6-32 as

$$\psi_1(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$$

The probability that the electron would be found in the region specified is

$$\int_0^{L/4} P_1(x) dx = \int_0^{L/4} \frac{2}{L} \sin^2 \left( \frac{\pi x}{L} \right) dx$$

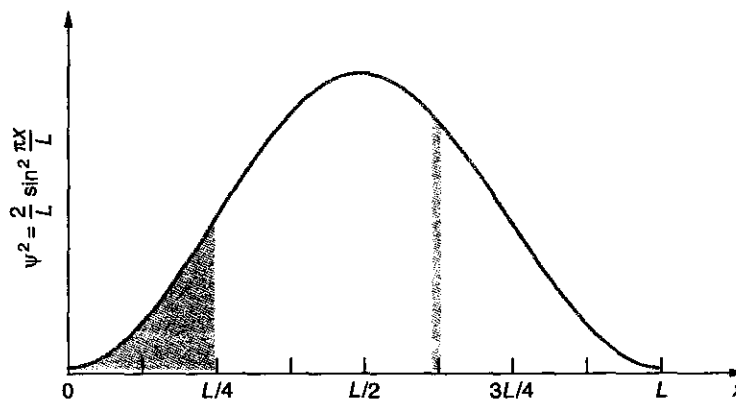
Letting  $u = \pi x/L$ , hence  $dx = L du/\pi$ , and noting the appropriate change in the limits on the integral, we have that

$$\int_0^{\pi/4} \frac{2}{\pi} \sin^2 u du = \frac{2}{\pi} \left( \frac{u}{2} - \frac{\sin 2u}{4} \right) \Big|_0^{\pi/4} = \frac{2}{\pi} \left( \frac{\pi}{8} - \frac{1}{4} \right) = 0.091$$

Thus, if one looked for the particle in a large number of identical searches, the electron would be found in the region  $0 < x < 0.25 \text{ cm}$  about 9 percent of



Fig. 6-6 The probability density  $\psi^2(x)$  vs.  $x$  for a particle in the ground state of an infinite square well potential. The probability of finding the particle in the region  $0 < x < L/4$  is represented by the larger shaded area. The narrow shaded band illustrates the probability of finding the particle within  $\Delta x = 0.01L$  around the point where  $x = 5L/8$ .



the time. This probability is illustrated by the shaded area on the left side in Figure 6-6.

(b) Since the region  $\Delta x = 0.01L$  is very small compared with  $L$ , we do not need to integrate, but can calculate the approximate probability as follows:

$$P = P(x)\Delta x = \frac{2}{L} \sin^2 \frac{\pi x}{L} \Delta x$$

Substituting  $\Delta x = 0.01L$  and  $x = 5L/8$ , we obtain

$$\begin{aligned} P &= \frac{2}{L} \sin^2 \frac{\pi(5L/8)}{L} (0.01L) \\ &= \frac{2}{L} (0.854)(0.01L) = 0.017 \end{aligned}$$

This means that the probability of finding the electron within  $0.01L$  around  $x = 5L/8$  is about 1.7 percent. This is illustrated in Figure 6-6, where the area of the shaded narrow band at  $x = 5L/8$  is 1.7 percent of the total area under the curve.

**EXAMPLE 6-4 An Electron in an Atomic-Size Box** (a) Find the energy in the ground state of an electron confined to a one-dimensional box of length  $L = 0.1 \text{ nm}$ . (This box is roughly the size of an atom.) (b) Make an energy-level diagram and find the wavelengths of the photons emitted for all transitions beginning at state  $n = 3$  and ending at a lower energy state.

### Solution

(a) The energy in the ground state is given by Equation 6-25. Multiplying the numerator and denominator by  $c^2/4\pi^2$ , we obtain an expression in terms of  $hc$  and  $mc^2$ , the energy equivalent of the electron mass (see Chapter 2):

$$E_1 = \frac{(hc)^2}{8mc^2L^2}$$

Substituting  $hc = 1240 \text{ eV} \cdot \text{nm}$  and  $mc^2 = 0.511 \text{ MeV}$ , we obtain

$$E_1 = \frac{(1240 \text{ eV} \cdot \text{nm})^2}{8(5.11 \times 10^5 \text{ eV})(0.1 \text{ nm})^2} = 37.6 \text{ eV}$$

This is of the same order of magnitude as the kinetic energy of the electron in the ground state of the hydrogen atom, which is 13.6 eV. In that case, the wavelength of the electron equals the circumference of a circle of radius 0.0529 nm, or about 0.33 nm, whereas for the electron in a one-dimensional box of length 0.1 nm, the wavelength in the ground state is  $2L = 0.2 \text{ nm}$ .

(b) The energies of this system are given by

$$E_n = n^2 E_1 = n^2 (37.6 \text{ eV})$$

Figure 6-7 shows these energies in an energy-level diagram. The energy of the first excited state is  $E_2 = 4(37.6 \text{ eV}) = 150.4 \text{ eV}$ , and that of the second excited state is  $E_3 = 9(37.6 \text{ eV}) = 338.4 \text{ eV}$ . The possible transitions from level 3 to level 2, from level 3 to level 1, and from level 2 to level 1 are indicated by the vertical arrows on the diagram. The energies of these transitions are

$$\Delta E_{3 \rightarrow 2} = 338.4 \text{ eV} - 150.4 \text{ eV} = 188 \text{ eV}$$

$$\Delta E_{3 \rightarrow 1} = 338.4 \text{ eV} - 37.6 \text{ eV} = 300.8 \text{ eV}$$

$$\Delta E_{2 \rightarrow 1} = 150.4 \text{ eV} - 37.6 \text{ eV} = 112.8 \text{ eV}$$

The photon wavelengths for these transitions are

$$\lambda_{3 \rightarrow 2} = \frac{hc}{\Delta E_{3 \rightarrow 2}} = \frac{1240 \text{ eV} \cdot \text{nm}}{188 \text{ eV}} = 6.60 \text{ nm}$$

$$\lambda_{3 \rightarrow 1} = \frac{hc}{\Delta E_{3 \rightarrow 1}} = \frac{1240 \text{ eV} \cdot \text{nm}}{300.8 \text{ eV}} = 4.12 \text{ nm}$$

$$\lambda_{2 \rightarrow 1} = \frac{hc}{\Delta E_{2 \rightarrow 1}} = \frac{1240 \text{ eV} \cdot \text{nm}}{112.8 \text{ eV}} = 11.0 \text{ nm}$$

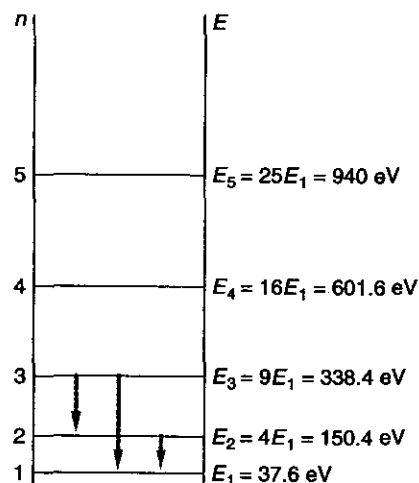


Fig. 6-7 Energy-level diagram for Example 6-4. Transitions from the state  $n = 3$  to the states  $n = 2$  and  $n = 1$ , and from the state  $n = 2$  to  $n = 1$ , are indicated by the vertical arrows.

### 6-3 The Finite Square Well

The quantization of energy that we found for a particle in an infinite square well is a general result that follows from the solution of the Schrödinger equation for any particle confined in some region of space. We shall illustrate this by considering the qualitative behavior of the wave function for a slightly more general potential energy function, the finite square well shown in Figure 6-8. The solutions of the Schrödinger equation for this type of potential energy are quite different, depending on whether the total energy  $E$  is greater or less than  $V_0$ . We shall defer discussion of the case  $E > V_0$  to Section 6-5 except to remark that in that case the particle is not confined and any value of the energy is allowed, i.e., there is no energy quantization. Here we shall assume that  $E < V_0$ .

Inside the well,  $V(x) = 0$  and the time-independent Schrödinger equation (Equation 6-18) becomes Equation 6-26, the same as for the infinite well:

$$\psi''(x) = -k^2\psi(x) \quad k^2 = \frac{2mE}{\hbar^2}$$

The solutions are sines and cosines (Equation 6-28) except that now we do not require  $\psi(x)$  to be zero at the well boundaries, but rather we require that  $\psi(x)$  and  $\psi'(x)$  be continuous at these points. Outside the well, i.e., for  $0 > x > L$ , Equation 6-18 becomes

$$\psi''(x) = \frac{2m}{\hbar^2}(V_0 - E)\psi(x) = \alpha^2\psi(x) \quad 6-33$$

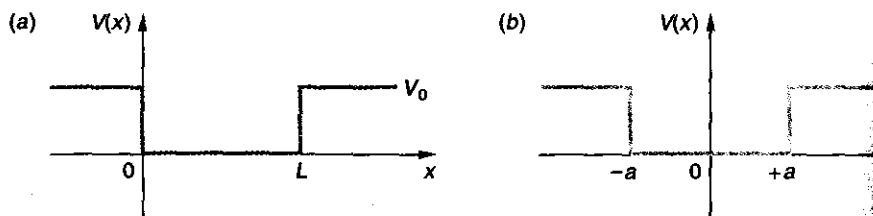
where

$$\alpha^2 = \frac{2m}{\hbar^2}(V_0 - E) > 0 \quad 6-34$$

The straightforward method of finding the wave functions and allowed energies for this problem is to solve Equation 6-33 for  $\psi(x)$  outside the well and then require that  $\psi(x)$  and  $\psi'(x)$  be continuous at the boundaries. The solution of Equation 6-33 is not difficult (it is of the form  $\psi(x) = Ce^{-\alpha x}$  for positive  $x$ ), but applying the boundary conditions involves a method that may be new to you; we describe it in the More on section on the Graphical Solution of the Finite Square Well.

First, we will explain in words unencumbered by the mathematics how the conditions of continuity of  $\psi$  and  $\psi'$  at the boundaries and the need for  $\psi \rightarrow 0$  as  $x \rightarrow \pm\infty$  lead to the selection of only certain wave functions and quantized energies for values of  $E$  within the well, i.e.,  $0 < E < V_0$ . The important feature of Equation 6-33 is that the second derivative  $\psi''$ , which is the curvature of the wave function, has the same sign

Fig. 6-8 (a) The finite square well potential. (b) The finite well arranged symmetrically about  $x = 0$ . Region I is that with  $x < -a$ , II with  $-a < x < +a$ , and III with  $x > +a$ .



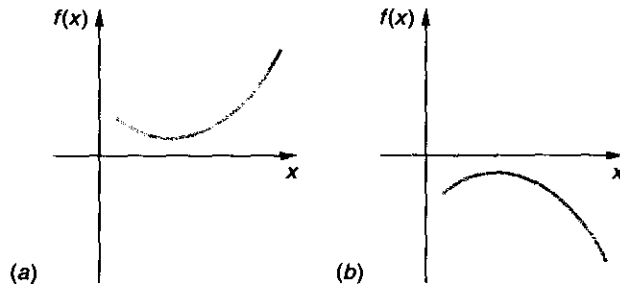
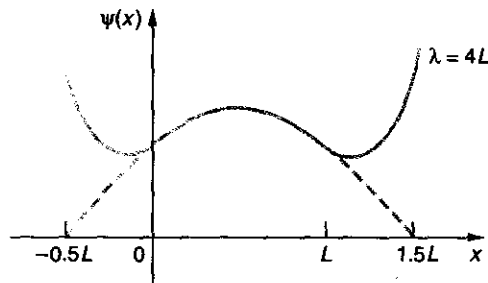


Fig. 6-9 (a) Positive function with positive curvature; (b) negative function with negative curvature.

the wave function  $\psi$ . If  $\psi$  is positive,  $\psi''$  is also positive and the wave function curves away from the axis, as shown in Figure 6-9a. Similarly, if  $\psi$  is negative,  $\psi''$  is negative and again,  $\psi$  curves away from the axis. This behavior is different from that inside the well, where  $0 < x < L$ . There,  $\psi$  and  $\psi''$  have opposite signs so that  $\psi$  always curves toward the axis like a sine or cosine function. Because of this behavior outside the well, for most values of the energy the wave function becomes infinite as  $x \rightarrow \pm\infty$ , i.e.,  $\psi(x)$  is not well behaved. Such functions, though satisfying the Schrödinger equation, are not proper wave functions because they cannot be normalized.

Figure 6-10 shows the wave function for the energy  $E = p^2/2m = \hbar^2/2m\lambda^2$  for  $\lambda = 4L$ . Figure 6-11 shows a well-behaved wave function corresponding to wavelength  $\lambda = \lambda_1$ , which is the ground-state wave function for the finite well, and the behavior of the wave functions for two nearby energies and wavelengths. The exact determination of the allowed energy levels in a finite square well can be obtained from a detailed solution of the problem. Figure 6-12 shows the wave functions and the probability distributions for the ground state and for the first two excited states. From this figure we see that the wavelengths inside the well are slightly longer than the corresponding wavelengths for the infinite well of the same width, so the corresponding energies are slightly less than those of the infinite well. Another feature of the finite well problem is that there are only a finite number of allowed energies, that number depending of the size of  $V_0$ . For very small  $V_0$  there is only one allowed energy level, i.e., only one bound state can exist. This will be quite apparent in the detailed solution in the More section.



6-10 The function that satisfies the Schrödinger equation with  $\lambda = 4L$  inside the well is not an acceptable wave function because it becomes infinite at large  $x$ . Although at  $x = L$  the function is heading toward zero (slope is negative), the rate of increase of the slope  $\psi''$  is so great that the slope becomes positive before the function becomes zero, and the function then increases without bound. Since  $\psi''$  has the same sign as  $\psi$ , the slope always increases and the function increases without bound. [This computer-generated plot courtesy of Paul Doherty, The Laboratory.]

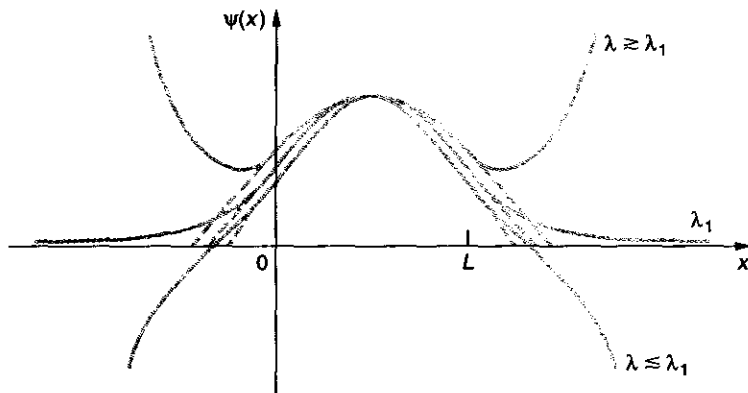


Fig. 6-11 Functions satisfying the Schrödinger equation with wavelengths near the critical wavelength  $\lambda_1$ . If  $\lambda$  is slightly greater than  $\lambda_1$ , the function approaches infinity like that in Figure 6-10. At the wavelength  $\lambda_1$ , the function and its slope approach zero together. This is an acceptable wave function corresponding to the energy  $E_1 = h^2/2m\lambda_1^2$ . If  $\lambda$  is slightly less than  $\lambda_1$ , the function crosses the  $+x$  axis while the slope is still negative. The slope becomes more negative because its rate of change  $\psi'$  is now negative. This function approaches negative infinity at large  $x$ . [This computer-generated plot courtesy of Paul Doherty, *The Exploratorium*.]

Note that, in contrast to the classical case, there is some probability of finding the particle outside the well, in the regions  $x > L$  or  $x < 0$ . In these regions, the total energy is less than the potential energy, so it would seem that the kinetic energy must be negative. Since negative kinetic energy has no meaning in classical physics, it is interesting to speculate about the meaning of this penetration of wave function beyond the well boundary. Does quantum mechanics predict that we could measure a negative kinetic energy? If so, this would be a serious defect in the theory. Fortunately, we are saved by the uncertainty principle. We can understand this qualitatively as follows (we shall consider the region  $x > L$  only). Since the wave function decreases as  $e^{-\alpha x}$ , with  $\alpha$  given by Equation 6-34, the probability density  $\psi^2 = e^{-2\alpha x}$  becomes very small in a distance of the order of  $\Delta x \approx \alpha^{-1}$ . If we consider  $\psi(x)$  to

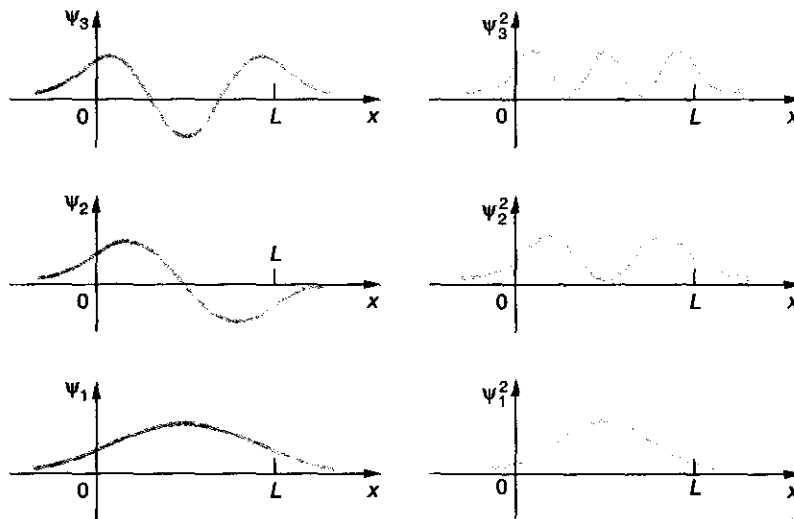


Fig. 6-12 Wave functions  $\psi_n(x)$  and probability distributions  $\psi_n^2(x)$  for  $n = 1, 2$ , and 3 for the finite square well. Compare these with Figure 6-4 for the infinite square well, where the wave functions are zero at  $x = 0$  and  $x = L$ . The wavelengths are slightly longer than the corresponding ones for the infinite well, so the allowed energies are somewhat smaller.

negligible beyond  $x = L + \alpha^{-1}$ , we can say that finding the particle in the region  $x > L$  is roughly equivalent to localizing it in a region  $\Delta x \approx \alpha^{-1}$ . Such a measurement introduces an uncertainty in momentum of the order of  $\Delta p \approx \hbar/\Delta x = \hbar\alpha$  and a minimum kinetic energy of the order of  $(\Delta p)^2/2m = \hbar^2\alpha^2/2m = V_0 - E$ . This kinetic energy is just enough to prevent us from measuring a negative kinetic energy! The penetration of the wave function into a classically forbidden region does have important consequences in tunneling or barrier penetration, which we shall discuss in Section 6-6.

Much of our discussion of the finite well problem applies to any problem in which  $E > V(x)$  in some region and  $E < V(x)$  outside that region. Consider, for example, the potential energy  $V(x)$  shown in Figure 6-13. Inside the well, the Schrödinger equation is of the form

$$\psi''(x) = -k^2\psi(x) \quad 6-35$$

where  $k^2 = 2m[E - V(x)]/\hbar^2$  now depends on  $x$ . The solutions of this equation are no longer simple sine or cosine functions because the wave number  $k = 2\pi/\lambda$  varies with  $x$ , but since  $\psi''$  and  $\psi$  have opposite signs,  $\psi$  will always curve toward the axis and the solutions will oscillate. Outside the well,  $\psi$  will curve away from the axis so there will be only certain values of  $E$  for which solutions exist that approach zero as  $x$  approaches infinity.

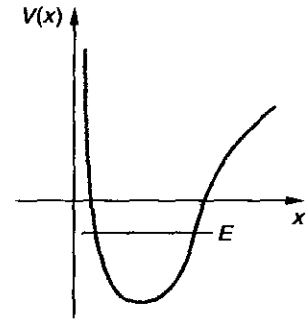


Fig. 6-13 Arbitrary well-type potential with possible energy  $E$ . Inside the well [ $E > V(x)$ ],  $\psi(x)$  and  $\psi''(x)$  have opposite signs, and the wave function will oscillate. Outside the well,  $\psi(x)$  and  $\psi''(x)$  have the same sign and, except for certain values of  $E$ , the wave function will not be well behaved.

## More

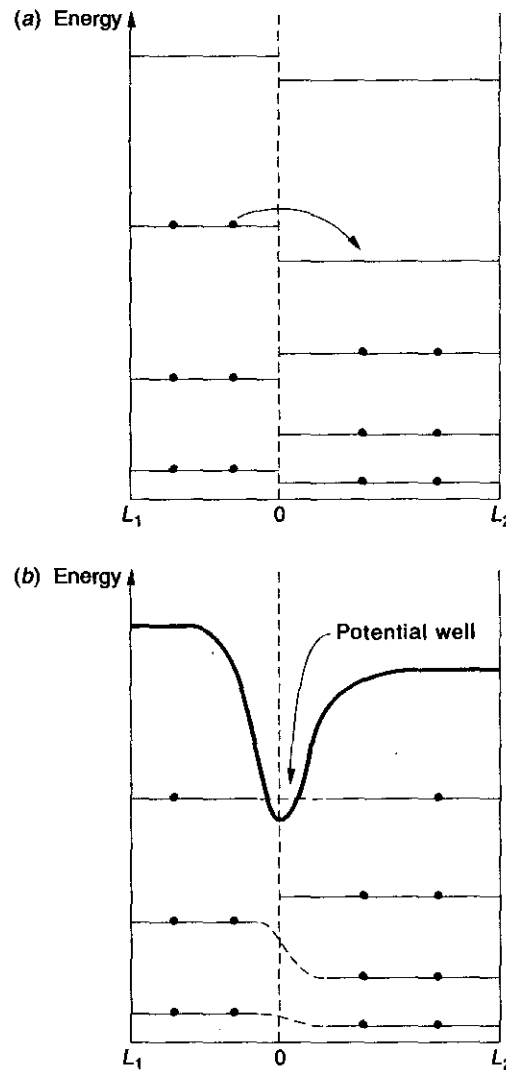
In most cases the solution of finite well problems involves transcendental equations and is very difficult. For some finite potentials, however, graphical solutions are relatively simple and provide both insights and numerical results. As an example, we have included the *Graphical Solution of the Finite Square Well* on the home page: [www.whfreeman.com/modphysics4e](http://www.whfreeman.com/modphysics4e) See also Equations 6-36 through 6-43 and Figure 6-14 here.

## Quantum Wells

Development of techniques for fabricating devices whose dimensions are of the order of nanometers, called *nanostuctures*, has enabled the construction of *quantum wells*. These are finite potential wells of one, two, and three dimensions that can channel electron movement in selected directions or, in the case of three-dimensional wells, called *quantum dots*, restrict electrons to quantized energy states within the well. They have potential applications in data storage and *quantum computers*, devices that greatly enhance computing power and speed.

One-dimensional quantum wells, called *quantum wires*, offer the possibility of dramatically increasing the speed at which electrons move through a device in selected directions. This in turn would increase the speed with which signals move between circuit elements in computer systems. Figure 6-15 is an outline of how such a well might be formed.

Fig. 6-15 (a) Two infinite square wells of different widths  $L_1$  and  $L_2$ , each containing the same number of electrons, are put together. An electron from well 1 moves to the lowest empty level of well 2. (b) The energies of the two highest electrons are equalized, but the unequal charge in the two wells distorts the energy-level structure. The distortion of the lowest empty levels in each well results in a potential well at the junction between the wells. The orientation of the newly formed well is perpendicular to the plane of the figure.



## 6-4 Expectation Values and Operators

### Expectation Values

The objective of theory is to explain experimental observations. In classical mechanics the solution of a problem is typically specified by giving the position of a particle or particles as a function of time. As we have discussed, the wave nature of matter prevents us from doing this for microscopic systems. Instead, we find the wave function  $\Psi(x, t)$  and the probability distribution function  $|\Psi(x, t)|^2$ . The most that we know about a particle's position is the probability that a measurement will yield various values of  $x$ . The *expectation value* of  $x$  is defined as

$$\langle x \rangle = \int_{-\infty}^{+\infty} \Psi^*(x, t) x \Psi(x, t) dx$$

The expectation value of  $x$  is the average value of  $x$  that we would expect to obtain from a measurement of the positions of a large number of particles with the same wave function  $\Psi(x, t)$ . As we have seen, for a particle in a state of definite energy the probability distribution is independent of time. The expectation value of  $x$  is then given by

$$\langle x \rangle = \int_{-\infty}^{+\infty} \Psi^*(x) x \Psi(x) dx \quad 6-45$$

For example, for the infinite square well, we can see by symmetry (or by direct calculation) that  $\langle x \rangle$  is  $L/2$ , the midpoint of the well.

In general, the expectation value of any function  $f(x)$  is given by

$$\langle f(x) \rangle = \int_{-\infty}^{+\infty} \Psi^* f(x) \Psi dx \quad 6-46$$

For example,  $\langle x^2 \rangle$  can be calculated as above, for the infinite square well of width  $L$ . It is left as an exercise to show that

$$\langle x^2 \rangle = \frac{L^2}{3} - \frac{L^2}{2n^2\pi^2} \quad 6-47$$

We should note that we don't necessarily expect to make a measurement whose result equals the expectation value. For example, for even  $n$ , the probability of measuring  $x = L/2$  in some range  $dx$  around the midpoint of the well is zero because the wave function  $\sin(n\pi x/L)$  is zero there. We get  $\langle x \rangle = L/2$  because the probability function  $\Psi^*\Psi$  is symmetrical about that point.

### Operators

If we knew the momentum  $p$  of a particle as a function of  $x$ , we could calculate the expectation value  $\langle p \rangle$  from Equation 6-46. However, it is impossible in principle to find  $p$  as a function of  $x$  since, according to the uncertainty principle, both  $p$  and  $x$  cannot be determined at the same time. To find  $\langle p \rangle$  we need to know the distribution function for momentum. If we know  $\Psi(x)$ , it can be found by Fourier analysis. It can be shown that  $\langle p \rangle$  can be found from

$$\langle p \rangle = \int_{-\infty}^{+\infty} \Psi^* \left( \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi dx \quad 6-48$$

Similarly,  $\langle p^2 \rangle$  can be found from

$$\langle p^2 \rangle = \int_{-\infty}^{+\infty} \Psi^* \left( \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \left( \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi dx$$

Note that in computing the expectation value the operator representing the physical quantity operates on  $\Psi(x, t)$ , not on  $\Psi^*(x, t)$ ; i.e., its correct position is between  $\Psi^*$  and  $\Psi$ . This is not important to the outcome when the operator is simply some constant, but it is critical when the operator includes a differentiation, as in the case of the momentum operator.



EXAMPLE 6-5 Expectation Values for  $p$  and  $p^2$  Find  $\langle p \rangle$  and  $\langle p^2 \rangle$  for the ground-state wave function of the infinite square well. (Before we calculate them, what do you think the results will be?)

### Solution

We can ignore the time dependence of  $\Psi$ , in which case we have

$$\begin{aligned}\langle p \rangle &= \int_0^L \left( \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \right) \left( \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \left( \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \right) dx \\ &= \frac{\hbar}{i} \frac{2}{L} \frac{\pi}{L} \int_0^L \sin \frac{\pi x}{L} \cos \frac{\pi x}{L} dx = 0\end{aligned}$$

The particle is equally as likely to be moving in the  $-x$  as in the  $+x$  direction, so its *average* momentum is zero.

Similarly, since

$$\begin{aligned}\frac{\hbar}{i} \frac{\partial}{\partial x} \left( \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \psi &= -\hbar^2 \frac{\partial^2 \psi}{\partial x^2} = -\hbar^2 \left( -\frac{\pi^2}{L^2} \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \right) \\ &= +\frac{\hbar^2 \pi^2}{L^2} \psi\end{aligned}$$

we have

$$\langle p^2 \rangle = \frac{\hbar^2 \pi^2}{L^2} \int_0^L \psi^* \psi dx = \frac{\hbar^2 \pi^2}{L^2} \int_0^L \psi^* \psi dx = \frac{\hbar^2 \pi^2}{L^2}$$

Note that  $\langle p^2 \rangle$  is simply  $2mE$  since, for the infinite square well,  $E = p^2/2m$ . The quantity  $(\hbar/i)\partial/\partial x$ , which operates on the wave function in Equation 6-48, is called the *momentum operator*  $p_{\text{op}}$ :

$$p_{\text{op}} = \frac{\hbar}{i} \frac{\partial}{\partial x} \quad 6-49$$

The time-independent Schrödinger equation (Equation 6-18) can be written conveniently in terms of  $p_{\text{op}}$ :

$$\left( \frac{1}{2m} \right) p_{\text{op}}^2 \psi(x) + V(x) \psi(x) = E \psi(x) \quad 6-50$$

where

$$p_{\text{op}}^2 \psi(x) = \frac{\hbar}{i} \frac{\partial}{\partial x} \left[ \frac{\hbar}{i} \frac{\partial}{\partial x} \psi(x) \right] = -\hbar^2 \frac{\partial^2 \psi}{\partial x^2}$$

In classical mechanics, the total energy written in terms of the position-momentum variables is called the Hamiltonian function  $H = p^2/2m + V$ . If we replace the momentum by the momentum operator  $p_{\text{op}}$  and note that  $V = V(x)$ , we obtain the Hamiltonian operator  $H_{\text{op}}$ :

$$H_{\text{op}} = \frac{p_{\text{op}}^2}{2m} + V(x) \quad 6-51$$

The time-independent Schrödinger equation can then be written

$$H_{\text{op}}\psi = E\psi \quad 6-52$$

The advantage of writing the Schrödinger equation in this formal way is that it allows for easy generalization to more complicated problems such as those with several particles moving in three dimensions. We simply write the total energy of the system in terms of position and momentum and replace the momentum variables by the appropriate operators to obtain the Hamiltonian operator for the system.

Table 6-1 summarizes the several operators representing physical quantities that we have discussed thus far and includes a few more that we will encounter later on.

TABLE 6-1 Some quantum-mechanical operators

Symbol	Physical quantity	Operator
$f(x)$	Any function of $x$ —e.g., the position $x$ , the potential energy $V(x)$ , etc.	$f(x)$
$p_x$	$x$ component of momentum	$\frac{\hbar}{i} \frac{\partial}{\partial x}$
$p_y$	$y$ component of momentum	$\frac{\hbar}{i} \frac{\partial}{\partial y}$
$p_z$	$z$ component of momentum	$\frac{\hbar}{i} \frac{\partial}{\partial z}$
$E$	Hamiltonian (time-independent)	$\frac{p_{\text{op}}^2}{2m} + V(x)$
$E$	Hamiltonian (time-dependent)	$i\hbar \frac{\partial}{\partial t}$
$E_k$	kinetic energy	$\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$
$L_z$	$z$ component of angular momentum	$-i\hbar \frac{\partial}{\partial \phi}$

#### QUESTIONS

Explain (in words) why  $\langle p \rangle$  and  $\langle p^2 \rangle$  in Example 6-5 are not both zero.

Can  $\langle x \rangle$  ever have a value that has zero probability of being measured?



## 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/modphysics4e](http://www.whfreeman.com/modphysics4e)) describes the process and applies it to the emission of light from an atom. See also Equations 6-52a-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.

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 with energy  $E$  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 potential energy. These points are called the classical turning points. The distance  $A$  is related to the total energy  $E$  by

$$E = \frac{1}{2}m\omega^2A^2 \quad 6-17$$

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

$$P_c(x) dx \propto \frac{dx}{v} = \frac{dx}{\sqrt{(2/m)(E - \frac{1}{2}m\omega^2x^2)}}$$

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

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + \frac{1}{2}m\omega^2x^2\psi(x) = E\psi(x)$$

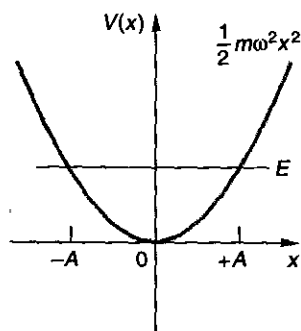


Fig. 6-17 Potential energy function for a simple harmonic oscillator. Classically, the particle with energy  $E$  is confined between the "turning points"  $-A$  and  $+A$ .

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 on "Parity"; see page 272.)

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

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

in

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

$\psi(x)$  curves away from the axis. Only certain values of  $E$  will lead to solutions that are well behaved, i.e., which 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

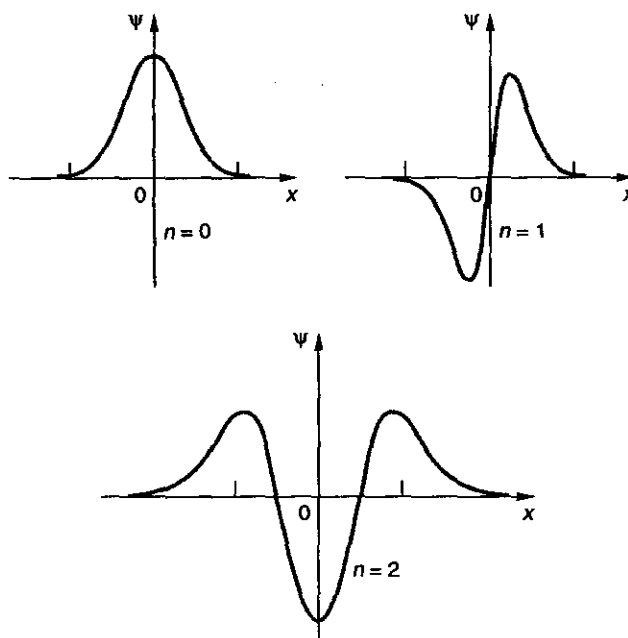
$$E_n = (n + \frac{1}{2})\hbar\omega \quad n = 0, 1, 2, \dots \quad 6-56$$

the ground-state energy is  $\frac{1}{2}\hbar\omega$  and the energy levels are equally spaced, each level 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  $E_0 = \frac{1}{2}\hbar\omega$  is the minimum energy consistent with the uncertainty principle. The allowed solutions to the Schrödinger equation, the wave functions for the simple harmonic oscillator, can be written

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

Fig. 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  $2$ .



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

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

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 and 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.

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

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

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 (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

$$\Delta n = \pm 1$$

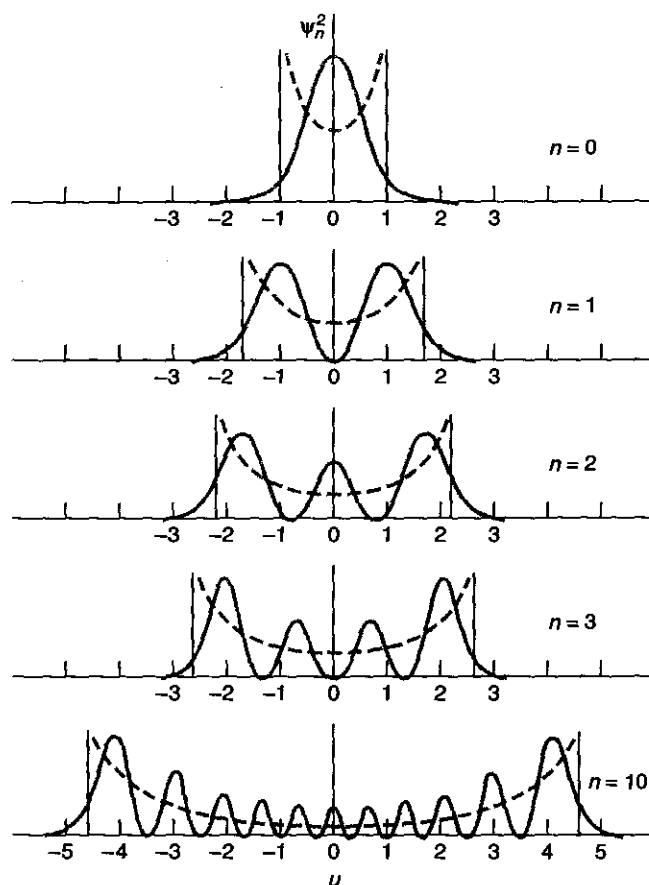


Fig. 6-19 Probability density  $\psi_n^2$  for the simple harmonic oscillator plotted against the dimensionless variable  $u = (m\omega/\hbar)^{1/2}x$ , for  $n = 0, 1, 2, 3$ , and  $10$ . The dashed curves are the classical probability densities for the same energy, and the vertical lines indicate the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

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.

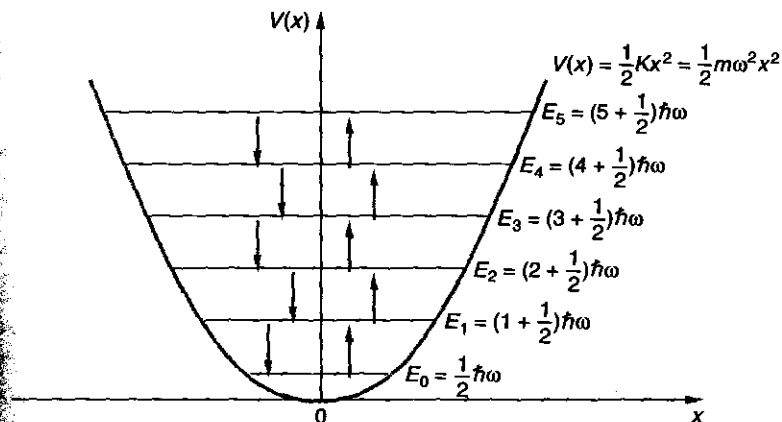


Fig. 6-20 Energy levels in the simple harmonic oscillator potential. Transitions obeying the selection rule  $\Delta n = \pm 1$  are indicated by the arrows (those pointing up indicate absorption). Since the levels have equal spacing, the same energy  $\hbar\omega$  is emitted or absorbed in all allowed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



## 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  $H_{\text{op}}$ , defined in Equation 6-51, is unchanged by a transformation that changes  $x \rightarrow -x$ . 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

$$H_{\text{op}}\psi(x) = E\psi(x) \quad 6-52$$

then a parity operation  $P$  leads to

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

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.,

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

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 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.

## 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 shall 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  $d^2\psi/dx^2$  and  $\psi(x)$  have opposite signs for those regions of  $x$  where  $E > V(x)$ , so  $\psi$

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 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  $lb - al < \infty$ . 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  $\rho$  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  $(b - a)$ .<sup>14</sup> The wave nature of the Schrödinger equation leads, when so, to some very interesting consequences.

### Step Potential

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

$$\begin{aligned} V(x) &= 0 & \text{for } x < 0 \\ V(x) &= V_0 & \text{for } x > 0 \end{aligned}$$

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. The classical answer is simple. For  $x < 0$ , each particle moves with speed  $v = (E/m)^{1/2}$ . 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 compare this classical problem as a ball rolling along a level surface and coming to a 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 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 is different when  $E > V_0$ , as in Figure 6-22a. The Schrödinger equation in each of the two space regions shown in the diagram is given by

Equation I

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

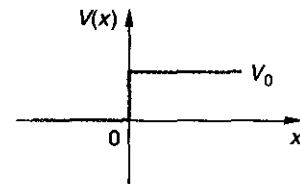
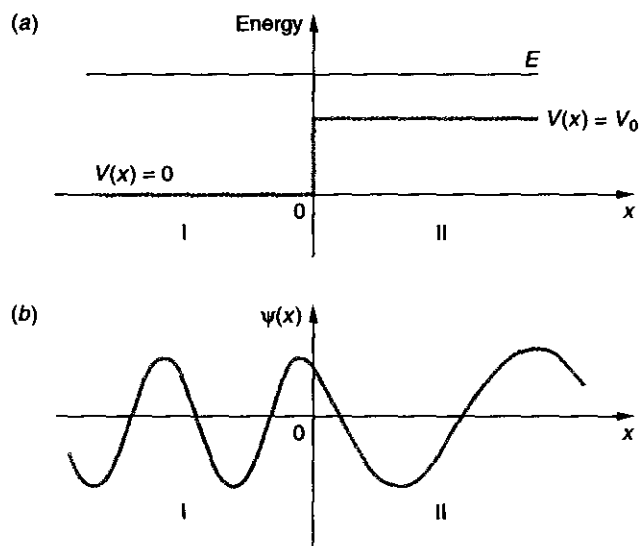


Fig. 6-21 Step potential. A classical particle incident from the left, with total energy  $E$  greater than  $V_0$ , is always transmitted. The potential change at  $x = 0$  merely provides an impulsive force which reduces the speed of the particle. A wave incident from the left is partially transmitted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



Fig. 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  $T < 1$ .



### Region II

$$(x > 0) \quad \frac{d^2\psi(x)}{dx^2} = -k_2^2\psi(x)$$

where

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

The general solutions are

### Region I

$$(x > 0) \quad \psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

### Region II

$$(x > 0) \quad \psi_{II}(x) = Ce^{ik_2x} + De^{-ik_2x}$$

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  $e^{-i\omega t}$ , yields a plane wave (i.e., a beam of free particles) moving to the right. The second term,  $Be^{-ik_1x}$ , represents particles moving to the left in Region I. In Equation 6-63,  $D = 0$ , 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 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  $d\psi/dx$  at  $x = 0$ .

requiring that  $\psi_I(0) = \psi_{II}(0)$  and  $d\psi(0)/dx = d\psi_{II}(0)/dx$ . Continuity of  $\psi$  at  $x = 0$  yields

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

or

$$A + B = C \quad 6-65a$$

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

$$k_1A - k_1B = k_2C \quad 6-65b$$

Solving Equations 6-65a and b for  $B$  and  $C$  in terms of  $A$  (see Problem 6-45), we have

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

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

Here 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  $A$ ,  $B$ , and  $C$  as<sup>15</sup>

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

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

in which it can be readily verified (see Problem 6-43) that

$$T + R = 1 \quad 6-70$$

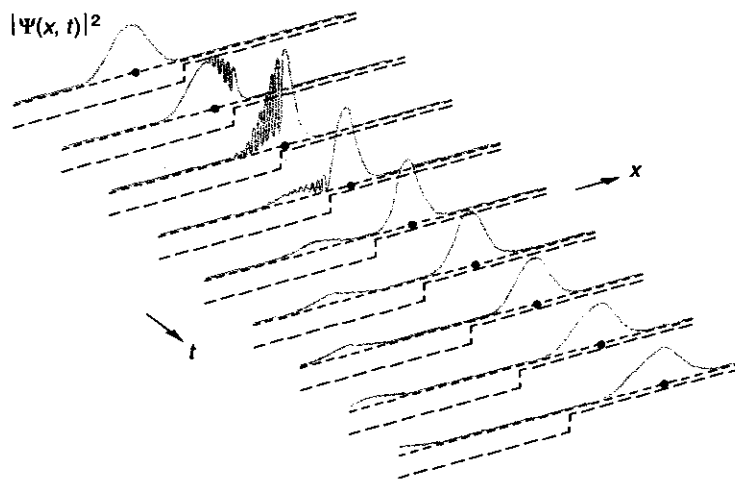
Among the interesting consequences of the wave nature of the solutions to Schrödinger's equation, notice the following:

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.)

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 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 6-22b

Fig. 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  $x = 0$ .



illustrates these points. Figure 6-23 shows the time development of a wave packet incident on a potential step for  $E > V_0$ .

Now let us consider the case shown in Figure 6-24a, 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,

$$\Psi_{II}(x) = Ce^{ik_2x} = Ce^{-\alpha x} \quad 6-67$$

is a *real* exponential function where  $\alpha = \sqrt{2m(V_0 - E)}/\hbar$ . (We choose the positive root so that  $\psi_{II} \rightarrow 0$  as  $x \rightarrow \infty$ .) This means that the numerator and denominator on the right side of Equation 6-66 are complex conjugates of one another, hence  $|B/A|^2$  and  $R = 1$  and  $T = 0$ . Figure 6-25 is a graph of both  $R$  and  $T$  versus energy of 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  $x = 0$ .

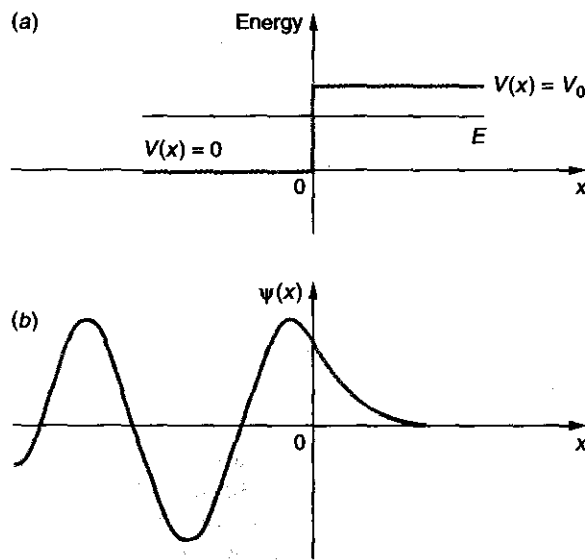


Fig. 6-24 (a) A potential step. Particles are incident on the step from the left moving toward the right, each with total energy  $E < V_0$ . (b) The wave transmitted into Region II is a decreasing exponential. However, the value of  $R$  in this case is 1 and no net energy is transmitted.

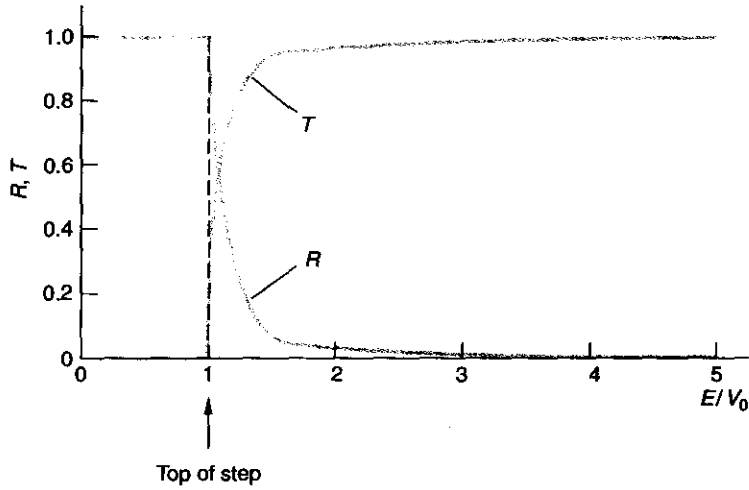


Fig. 6-25 Reflection coefficient  $R$  and transmission coefficient  $T$  for a potential step  $V_0$  high versus energy  $E$  (in units of  $V_0$ ).

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

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

Figure 6-24b 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 of 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 could be *measured* in such a region, because to locate the particle in such a region produces 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  $E = 0.1 V_0$ , are incident on a potential step with  $V_0 = 1$  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,

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

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  $2\alpha = 2[2m(0.9V_0)]^{1/2}/\hbar$ , the first two columns of Table 6-2. Multiplying  $e^{-2\alpha x}$  and then multiplying by  $|C|^2 = 0.4$  yield  $|\psi|^2$ , which is graphed in Figure 6-26.

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

$x$ (m)	$2\alpha x$	$ \psi ^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	$\approx 0$

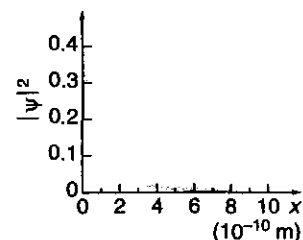


Fig. 6-26

### 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

$$V(x) = \begin{cases} V_0 & \text{for } 0 < x < a \\ 0 & \text{for } x < 0 \text{ and } x > a \end{cases} \quad 6-7$$

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, 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!

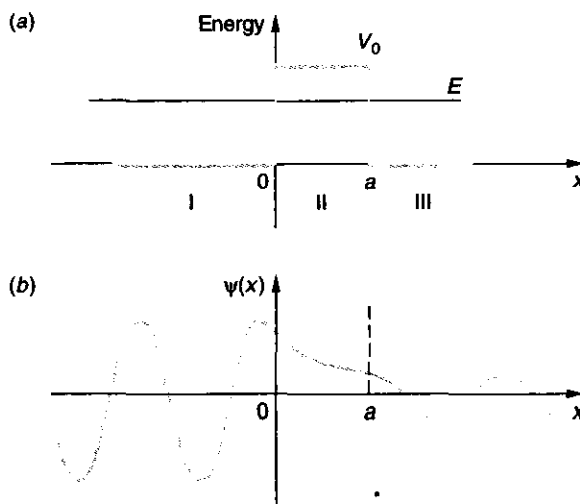


Fig. 6-27 (a) Square barrier potential. (b) Penetration of the barrier by a wave with energy less than the barrier energy. Part of the wave is transmitted by the barrier even though, classically, the particle cannot enter the region  $0 < x < a$  in which the potential energy is greater than the total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

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, is incident from the left. The general solutions to the wave equation are, following the example of the potential step,

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

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 6-27b. This implies that there will be some probability of the particles represented by the wave function being found on the far right outside of the 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 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 (Problem 6-61)

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

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

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

**Scanning Tunneling Microscope** In the *scanning tunneling microscope (STM)*, developed in the 1980s by Gerd Binnig and Heinrich Rohrer, a narrow gap between a conducting specimen and the tip of a tiny probe acts as a potential barrier to electrons 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 joining 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

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.

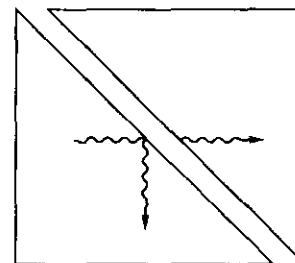
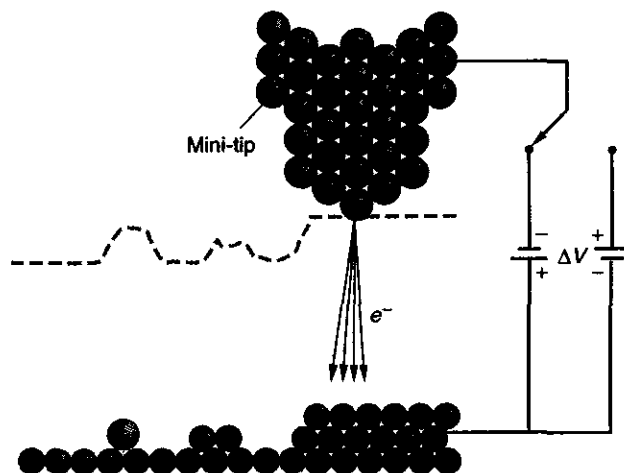


Fig. 6-28 Optical barrier penetration, sometimes called frustrated total internal reflection. Because of the presence of the second prism, part of the wave penetrates the air barrier even though the angle of incidence in the first prism is greater than the critical angle. This effect can be demonstrated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

Fig. 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 micro-tip 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.



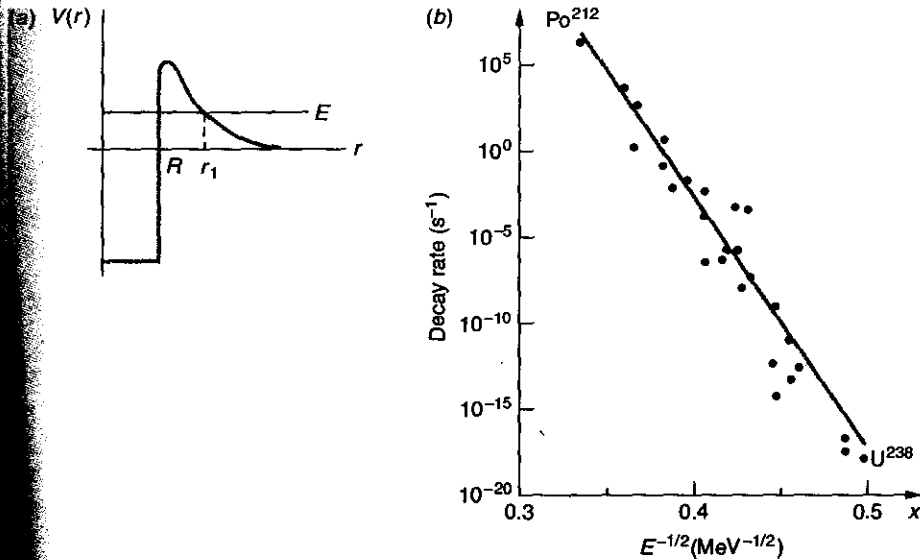
surface features of a specimen can be measured by STMs with a resolution of the order of the size of a single atom.

Scanning tunneling microscopes (STMs) have the disadvantage of requiring a conducting surface for their operation. This problem is avoided in atomic force microscopes (AFMs) that track the sample surface by maintaining a constant interatomic force between the atoms on the scanner tip and the sample's surface atoms. In this AFM image of actin filaments from contractile myofibrils in skeletal muscle the 8-nm width of the filaments is clearly resolved. [Taken from [www.di.com](http://www.di.com), of Digital Instruments, Veeco Metrology Group, Santa Barbara, CA.]



## Exploring Alpha Decay

Barrier penetration was used by Gamow, Condon, and Gurney in 1928 to explain the enormous variation in the mean life for  $\alpha$  decay of radioactive nuclei and the seemingly paradoxical very existence of  $\alpha$  decay.<sup>16</sup> While radioactive  $\alpha$  decay will be discussed more thoroughly in Chapter 11, in general the smaller the energy of the  $\alpha$  particle, the larger the mean life. The energies of  $\alpha$  particles from natural radioactive sources range from about 4 to 9 MeV, whereas the mean lifetimes range



6-30 (a) Model of potential energy function for an  $\alpha$  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  $2e$  is the charge of the  $\alpha$  particle. An  $\alpha$  particle inside the nucleus oscillates back and forth, being reflected at the barrier at  $R$ . Because of its wave properties, when the  $\alpha$  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 6-27b. (b) The decay rate for the emission of  $\alpha$  particles from radioactive nuclei. The solid curve is the prediction of Equation 6-79; the points are experimental results.

out  $10^{10}$  years to  $10^{-6}$  s. Gamow represented the radioactive nucleus by a potential well containing an  $\alpha$  particle, as shown in Figure 6-30a. For  $r$  less than the nuclear radius  $R$ , the  $\alpha$  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  $\alpha$  particle is repelled by the Coulomb force. This is represented by the Coulomb potential energy  $+kZze^2/r$ , where  $z = 2$  for the  $\alpha$  particle and  $Ze$  is the remaining nuclear charge. The energy  $E$  is the measured kinetic energy of the emitted particle, since when it is far from the nucleus its potential energy is zero. We see in the figure that a small increase in  $E$  reduces the relative height of the barrier above  $E$  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, which in turn leads to a shorter lifetime. Gamow and his co-workers were able to derive an expression for the  $\alpha$  decay rate and the mean lifetime as a function of energy  $E$  that is in good agreement with experimental results as follows:

The probability that an  $\alpha$  particle will tunnel through the barrier in any one attempt 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

$$T \approx e^{-2\sqrt{2m(V_0-E)}ah} \quad 6-77$$

is a very small number, i.e., the  $\alpha$  particle is usually reflected. The number of attempts per second  $N$  that the  $\alpha$  particle approaches the barrier is given approximately by



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

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

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  $\alpha$  particle, which is also the reciprocal of the mean life  $\tau$ , is given by

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

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



## Exploring *NH<sub>3</sub> Atomic Clock*

Barrier penetration also takes place in the case of the periodic *inversion* of the ammonia molecule. The  $\text{NH}_3$  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, 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.<sup>17</sup> The oscillation frequency  $f = 2.3786 \times 10^{10}$  Hz when the atom in the state characterized by the energy  $E_1$  in Figure 6-31*b*. This frequency is quite low compared with those of most molecular vibrations, a fact that allowed the N atom tunneling frequency in  $\text{NH}_3$  to be used as the standard in the first *atomic clocks*, devices that now provide the world's standard for precision timekeeping.

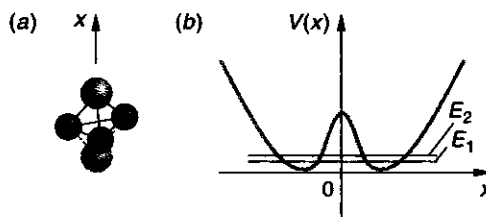


Fig. 6-31 (a) The  $\text{NH}_3$  molecule oscillates between the two equilibrium positions shown; the H atoms form a plane; the N atom is colored. (b) The potential energy of the N atom,  $V(x)$ , as a function of the distance  $x$  above and below the plane of the H atoms. Several of the allowed energy levels, 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/modphysics4e](http://www.whfreeman.com/modphysics4e) See also Equation 6-80 and Figure 6-32 here.

## Summary

TOPIC	RELEVANT EQUATIONS AND REMARKS	
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
Time independent, one space dimension	$\frac{-\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$	6-18
Normalization condition	$\int_{-\infty}^{+\infty} \Psi^*(x, t)\Psi(x, t) dx = 1$	6-9
	and	
	$\int_{-\infty}^{+\infty} \psi^*(x)\psi(x) dx = 1$	6-20
Acceptability conditions	<ol style="list-style-type: none"> <li>1. <math>\psi(x)</math> and <math>d\psi/dx</math> must be continuous.</li> <li>2. <math>\psi(x)</math> and <math>d\psi/dx</math> must be finite.</li> <li>3. <math>\psi(x)</math> and <math>d\psi/dx</math> must be single-valued.</li> <li>4. <math>\psi(x) \rightarrow 0</math> as <math>x \rightarrow \infty</math>.</li> </ol>	
Infinite square well		
Allowed energies	$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} \quad n = 1, 2, 3, \dots$	6-24
Wave functions	$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad n = 1, 2, 3, \dots$	6-32
Finite square well	For a finite well of width $L$ the allowed energies $E_n$ in the well are lower than the corresponding levels for an infinite well. There is always at least one allowed energy (bound state) in a finite well.	
Expectation values and operators	The expectation or average value of a physical quantity represented by an operator, such as the momentum operator $p_{op}$ , is given by	
	$\langle p \rangle = \int_{-\infty}^{+\infty} \psi^* p_{op} \psi dx = \int_{-\infty}^{+\infty} \psi^* \left( \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \psi dx$	6-48

Continued

## TOPIC

## RELEVANT EQUATIONS AND REMARKS

## 5. Simple harmonic oscillator

Allowed energies

$$E_n = (n + \frac{1}{2})\hbar\omega \quad n = 0, 1, 2, \dots$$

6-56

## 6. Reflection and transmission

When the potential changes abruptly in a distance small compared to the de Broglie wavelength, a particle may be reflected even though  $E > V(x)$ . A particle may also penetrate into a region where  $E < V(x)$ .

## GENERAL REFERENCES

The following general references are written at a level appropriate for the readers of this book.

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Mehra, J., and H. Rechenberg, *The Historical Development of Quantum Theory*, Vol. 1, Springer-Verlag, New York, 1982

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Visual Quantum Mechanics, Kansas State University, Manhattan, 1996. Computer simulation software allows the user to analyze a variety of one-dimensional potentials including the square wells and harmonic oscillator discussed in this chapter.

## NOTES

1. Felix Bloch (1905–1983), Swiss-American physicist. He was a student at the University of Zürich and attended the colloquium referred to. The quote is from an address before the American Physical Society in 1976. Bloch shared the 1952 Nobel Prize in physics for measuring the magnetic moment of the neutron, using a method that he invented that led to the development of the analytical technique of nuclear magnetic resonance (NMR) spectroscopy.

2. Peter J. W. Debye (1884–1966), Dutch-American physical chemist. He succeeded Einstein in the chair of theoretical physics at the University of Zürich and received the Nobel Prize in chemistry in 1936.

3. Erwin R. J. A. Schrödinger (1887–1961), Austrian physicist. He succeeded Planck in the chair of theoretical physics at the University of Berlin in 1928 following the latter's retirement and two years after publishing in rapid succession six papers that set forth the theory of wave mechanics. For that work he shared the physics Nobel Prize with P. A. M. Dirac in 1933. He left Nazi-controlled Europe in 1940, moving his household to Ireland.

4. To see that this is indeed the case, consider the effect on  $\partial^2\Psi(x, t)/\partial x^2$  of multiplying  $\Psi(x, t)$  by a factor  $C$ . Then  $\partial^2 C\Psi(x, t)/\partial x^2 = C\partial^2\Psi(x, t)/\partial x^2$ , and the derivative is increased by the same factor. Thus, the derivative is proportional to the first power of the function, i.e., it is linear in  $\Psi(x, t)$ .

5. The imaginary  $i$  appears because the Schrödinger equation relates a *first* time derivative to a *second* space derivative

as a consequence of the fact that the total energy is related to the *square* of the momentum. This is unlike the classical wave equation (Equation 5-11), which relates two *second* derivatives. The implication of this is that, in general,  $\Psi(x, t)$  will be complex functions, whereas the  $y(x, t)$  are real.

6. The fact that  $\Psi$  is in general complex does not mean its imaginary part doesn't contribute to the values of measurements, which are real. Every complex number can be written in the form  $z = a + bi$ , where  $a$  and  $b$  are real numbers and  $i = (-1)^{1/2}$ . The magnitude or absolute value is defined as  $(a^2 + b^2)^{1/2}$ . The complex conjugate of  $z$  is  $a - bi$ , so  $z^*z = (a - bi)(a + bi) = a^2 + b^2 = |z|^2$ ; the value of  $|\Psi|^2$  will contain a contribution from its imaginary part.

7. Here we are using the convention of probability statistics that certainty is represented by a probability of 1.

8. This method for solving partial differential equations called *separation of variables*, for obvious reasons, works for most potentials in quantum mechanics, as in classical mechanics, are time-independent, the method may be applied to the Schrödinger equation in numerous situations.

9. We should note that there is an exception to this rule in the quantum theory of measurement.

10.  $E = 0$  corresponding to  $n = 0$  is not a possible energy for a particle in a box. As discussed in Section 5-6, the uncertainty principle limits the minimum energy for such a particle to values  $> \hbar^2/2mL^2$ .

11. Recalling that linear combinations of solutions to Schrödinger's equation will also be solutions, we should note here that simulation of the classical behavior of a macroscopic particle in a macroscopic box requires wave functions that are the superpositions of many stationary states. Thus, the classical particle never has definite energy in the quantum-mechanical sense.

12. To simplify the notation in this section we shall sometimes omit the functional dependence and merely write  $\psi_n$  for  $\psi_n(x)$  and  $\Psi_n$  for  $\Psi_n(x, t)$ .

13. The Hermite polynomials are known functions which are tabulated in most books on quantum mechanics.

14. It is straightforward to show that the only difference between a  $\psi(x)$  normalized in terms of the particle density and one for which  $|\psi(x)|^2$  is the probability density is a multiplicative constant.

15.  $T$  and  $R$  are derived in terms of the particle currents, i.e., particles/unit time, in most introductory quantum mechanics books.

16. Rutherford had shown that the scattering of 8.8-MeV  $\alpha$  particles from the decay of  $^{212}\text{Po}$  obeyed the Coulomb force law down to distances of the order of  $3 \times 10^{-14}$  m, i.e., down to about nuclear dimensions. Thus, the Coulomb barrier at that distance was at least 8.8 MeV high; however, the energy of  $\alpha$  particles emitted by  $^{238}\text{U}$  is only 4.2 MeV, less than half the barrier height. How that could be possible presented classical physics with a paradox.

17. Since the molecule's center of mass is fixed in an inertial reference frame, the plane of H atoms also oscillates back and forth in the opposite direction to the N atom; however, their mass being smaller than that of the N atom, the amplitude of the plane's motion is actually larger than that of the N atom. It is the relative motion that is important.

18. See, for example, F. Capasso and S. Datta, "Quantum Electron Devices," *Physics Today*, **43**, 74 (1990). Leo Esaki was awarded the Nobel Prize in physics in 1973 for inventing the resonant tunnel diode.

## PROBLEMS

### Level 1

#### Problem 6-1 The Schrödinger Equation in One Dimension

Show that the wave function  $\Psi(x, t) = Ae^{kx - \omega t}$  does not satisfy the time-dependent Schrödinger equation.

Show that  $\Psi(x, t) = Ae^{i(kx - \omega t)}$  satisfies both the time-dependent Schrödinger equation and the classical wave equation (Equation 6-1).

In a region of space, a particle has a wave function given by  $\psi(x) = Ae^{-x^2/2L^2}$  and energy  $\hbar^2/2mL^2$ , where  $L$  is some length. (a) Find the potential energy as a function of  $x$ . Sketch  $V$  versus  $x$ . (b) What is the classical potential that has this dependence?

(a) For Problem 6-3, find the kinetic energy as a function of  $x$ . (b) Show that  $x = L$  is a classical turning point. (c) The potential energy of a simple harmonic oscillator in terms of its angular frequency  $\omega$  is given by  $V(x) = \frac{1}{2}m\omega^2x^2$ . Compare this with your answer to part (a) of Problem 6-3, and show that the total energy for this wave function can be written  $E = \frac{1}{2}\hbar\omega$ .

(a) Show that the wave function  $\Psi(x, t) = A \sin(kx - \omega t)$  does not satisfy the time-dependent Schrödinger equation. (b) Show that  $\Psi(x, t) = A \cos(kx - \omega t) + iA \sin(kx - \omega t)$  does satisfy this equation.

The wave function for a free electron, i.e., one on which no net force acts, is given by  $\psi(x) = A \sin(2.5 \times 10^{10} x)$  where  $x$  is in meters. Compute the electron's (a) momentum, (b) total energy, and (c) de Broglie wavelength.

A particle with mass  $m$  and total energy zero is in a particular region of space where its wave function is  $\psi(x) = Ce^{-x^2/2L^2}$ . (a) Find the potential energy  $V(x)$  versus  $x$ . Make a sketch of  $V(x)$  versus  $x$ .

Normalize the wave function in Problem 6-2 between  $-a$  and  $+a$ . Why can't that wave function be normalized between  $-\infty$  and  $+\infty$ ?

#### Problem 6-2 The Infinite Square Well

A particle is in an infinite square well of size  $L$ . Calculate the ground-state energy if the particle is a proton and  $L = 0.1$  nm, a typical size for a molecule; and (b) if the particle is a proton and  $L = 1$  fm, a typical size for a nucleus.

- 6-10. A particle is in the ground state of an infinite square well potential given by Equation 6-21. Find the probability of finding the particle in the interval  $\Delta x = 0.002 L$  at (a)  $x = L/2$ , (b)  $x = 2L/3$ , and (c)  $x = L$ . (Since  $\Delta x$  is very small, you need not do any integration.)
- 6-11. Do Problem 6-10 for particle in the second excited state ( $n = 3$ ) of an infinite square well potential.
- 6-12. A mass of  $10^{-6}$  g is moving with a speed of about  $10^{-1}$  cm/s in a box 1 cm in length. Treating this as a one-dimensional infinite square well, calculate the approximate value of the quantum number  $n$ .
- 6-13. (a) For the classical particle of Problem 6-12, find  $\Delta x$  and  $\Delta p$ , assuming that  $\Delta x/L = 0.01$  percent and  $\Delta p/p = 0.01$  percent. (b) What is  $(\Delta x \Delta p)/\hbar$ ?
- 6-14. A particle of mass  $m$  is confined to a tube of length  $L$ . (a) Use the uncertainty relationship to estimate the smallest possible energy. (b) Assume that the inside of the tube is a force-free region and that the particle makes elastic reflections at the tube ends. Use Schrödinger's equation to find the ground-state energy for the particle in the tube. Compare the answer to that of part (a).
- 6-15. (a) What is the wavelength associated with the particle of Problem 6-14 if the particle is in its ground state? (b) What is the wavelength if the particle is in its second excited state (quantum number  $n = 3$ )? (c) Use de Broglie's relationship to find the magnitude for the momentum of the particle in its ground state. (d) Show that  $p^2/2m$  gives the correct energy for the ground state of this particle in the box.
- 6-16. The wavelength of light emitted by a ruby laser is 694.3 nm. Assuming that the emission of a photon of this wavelength accompanies the transition of an electron from the  $n = 2$  level to the  $n = 1$  level of an infinite square well, compute  $L$  for the well.
- 6-17. Suppose a macroscopic bead with a mass of 2.0 g is constrained to move on a straight frictionless wire between two heavy stops clamped firmly to the wire 10 cm apart. If the bead is moving at a speed of 20 nm/yr (i.e., to all appearances it is at rest), what is the value of its quantum number  $n$ ?
- 6-18. An electron moving in a one-dimensional infinite square well is trapped in the  $n = 2$  state. (a) Show that the probability of finding the electron between  $x = 0.2 L$  and  $x = 0.4 L$  is  $1/5$ . (b) Compute the probability of finding the electron within the "volume"  $\Delta x = 0.002 L$  at  $x = L/2$ .
- 6-19. In the early days of nuclear physics before the neutron was discovered, it was thought that the nucleus contained only electrons and protons. If we consider a nucleus to be a one-dimensional infinite well with  $L = 10$  fm and ignore relativistic effects, compute the ground-state energy for (a) an electron and (b) a proton in the nucleus. (c) Compute the energy difference between the ground state and the first excited state for each particle. (Differences between energy levels in nuclei are found to be typically of the order of 1 MeV.)
- 6-20. An electron is in the ground state with energy  $E_n$  of a one-dimensional infinite square well with  $L = 10^{-10}$  m. Compute the force that the electron exerts on the wall during an impact on either wall. (Hint:  $F = -dE_n/dL$ . Why?) How does this result compare with the weight of an electron at the surface of Earth?
- 6-21. The wave functions of a particle in a one-dimensional infinite square well are given by Equation 6-32. Show that for these functions  $\int \psi_n(x) \psi_m(x) dx = 0$ , i.e., that  $\psi_n(x)$  and  $\psi_m(x)$  are orthogonal.

### Section 6-3 The Finite Square Well

- 6-22. Sketch (a) the wave function and (b) the probability distribution for the  $n = 4$  state of the finite square well potential.
- 6-23. Repeat Problem 6-22 for the  $n = 5$  state of the well.
- 6-24. An electron is confined to a finite square well whose "walls" are 8.0 eV high. If the ground-state energy is 0.5 eV, estimate the width of the well.

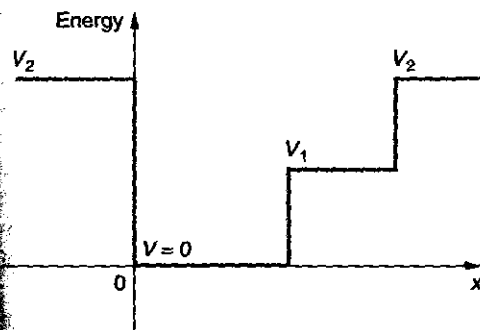


Fig. 6-33 Problem 6-25.

25. Using arguments concerning curvature, wavelength, and amplitude, sketch very carefully the wave function corresponding to a particle with energy  $E$  in the finite potential well shown in Figure 6-33.
26. For a finite square well potential that has six quantized levels, if  $a = 10$  nm (a) sketch the finite well, (b) sketch the wave function from  $x = -2a$  to  $x = +2a$  for  $n = 3$ , and (c) sketch the probability density for the same range of  $x$ .
27. The mass of the deuteron (the nucleus of the hydrogen isotope  $^2\text{H}$ ) is  $1.88 \text{ GeV}/c^2$ . How deep must a finite potential well be whose width is  $2 \times 10^{-15} \text{ m}$  if there are two energy levels in the well?

Section 6-4 Expectation Values and Operators

28. Find (a)  $\langle x \rangle$  and (b)  $\langle x^2 \rangle$  for the second excited state ( $n = 3$ ) in an infinite square well potential.
29. (a) Show that the classical probability distribution function for a particle in a one-dimensional infinite square well potential of length  $L$  is given by  $P(x) = 1/L$ . (b) Use your result in (a) to find  $\langle x \rangle$  and  $\langle x^2 \rangle$  for a classical particle in such a well.
30. Show directly from the time-independent Schrödinger equation that  $\langle p^2 \rangle = 2m\langle E - V(x) \rangle$  in general and that  $\langle p^2 \rangle = \langle 2mE \rangle$  for the infinite square well. Use this result to compute  $\langle p^2 \rangle$  for the ground state of the infinite square well.
31. Find  $\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ ,  $\sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$ , and  $\sigma_x \sigma_p$  for the ground-state wave function of an infinite square well. (Use the fact that  $\langle p \rangle = 0$  by symmetry and  $\langle p^2 \rangle = 2mE$  from Problem 6-30.)
32. Compute  $\langle x \rangle$  and  $\langle x^2 \rangle$  for the ground state of a harmonic oscillator (Equation 6-58).  $A_0 = (m\omega/\hbar\pi)^{1/4}$ .
33. Use conservation of energy to obtain an expression connecting  $x^2$  and  $p^2$  for a harmonic oscillator, then use it along with the result from Problem 6-32 to compute  $\langle p^2 \rangle$  for the harmonic oscillator ground state.
34. (a) Using  $A_0$  from Problem 6-32, write down the total wave function  $\Psi_0(x, t)$  for the ground state of a harmonic oscillator. (b) Use the operator for  $p_x$  from Table 6-1 to compute  $\langle p^2 \rangle$ .

Section 6-5 The Simple Harmonic Oscillator

35. For the harmonic oscillator ground state  $n = 0$  the Hermite polynomial  $H_n(x)$  in Equation 6-57 is given by  $H_0 = 1$ . Find (a) the normalization constant  $C_0$ , (b)  $\langle x^2 \rangle$ , and (c)  $\langle x \rangle$  for this state. (Hint: Use Table B1 to compute the needed integrals.)
36. For the first excited state,  $H_1(x) = x$ . Find (a) the normalization constant  $C_1$ , (b)  $\langle x \rangle$ , (c)  $\langle x^2 \rangle$ , (d)  $\langle V(x) \rangle$  for this state (see Problem 6-35).
37. A quantum harmonic oscillator of mass  $m$  is in the ground state with classical turning points at  $\pm A$ . (a) With the mass confined to the region  $\Delta x \approx 2A$ , compute  $\Delta p$  for this

state. (b) Compare the kinetic energy implied by  $\Delta p$  with (1) the ground-state total energy and (2) the expectation value of the kinetic energy.

6-38. Compute the spacing between adjacent energy levels per unit energy, i.e.,  $\Delta E_n/E_n$ , for the quantum harmonic oscillator and show that the result agrees with Bohr's correspondence principle (see Section 4-3) by letting  $n \rightarrow \infty$ .

6-39. The period of a macroscopic pendulum made with a mass of 10 g suspended from a massless cord 50 cm long is 1.42 s. (a) Compute the ground-state (zero-point) energy. (b) If the pendulum is set into motion so that the mass raises 0.1 mm above its equilibrium position, what will be the quantum number of the state? (c) What is the frequency of the motion in (b)?

6-40. Show that the wave functions for the ground state and the first excited state of the simple harmonic oscillator, given in Equation 6-58, are orthogonal, that is, show that  $\int \psi_0(x)\psi_1(x) dx = 0$ .

### Section 6-6 Reflection and Transmission of Waves

6-41. A free particle of mass  $m$  with wave number  $k_1$  is traveling to the right. At  $x = 0$  the potential jumps from zero to  $V_0$  and remains at this value for positive  $x$ . (a) If the total energy is  $E = \hbar^2 k_1^2 / 2m = 2V_0$ , what is the wave number  $k_2$  in the region  $x > 0$ ? Express your answer in terms of  $k_1$  and  $V_0$ . (b) Calculate the reflection coefficient  $R$  at the potential step. (c) What is the transmission coefficient  $T$ ? (d) If one million particles with wave number  $k_1$  are incident upon the potential step, how many particles are expected to continue along in the positive  $x$  direction? How does this compare with classical prediction?

6-42. In Problem 6-41, suppose that the potential jumps from zero to  $-V_0$  at  $x = 0$  so that the free particle speeds up instead of slowing down. The wave number for the incident particle is again  $k_1$ , and the total energy is  $2V_0$ . (a) What is the wave number for the particle in the region of positive  $x$ ? (b) Calculate the reflection coefficient  $R$  at the potential step. (c) What is the transmission coefficient  $T$ ? (d) If one million particles with wave number  $k_1$  are incident upon the potential step, how many particles are expected to continue along in the positive  $x$  direction? How does this compare with classical prediction?

6-43. Use Equations 6-68 and 6-69 to derive Equation 6-70.

6-44. For particles incident on a step potential with  $E < V_0$ , show that  $T = 0$  using Equation 6-70.

6-45. Derive Equations 6-66 and 6-67 from those that immediately precede them.

6-46. A beam of electrons, each with kinetic energy  $E = 2.0$  eV, is incident on a potential barrier with  $V_0 = 6.5$  eV and width  $5.0 \times 10^{-10}$  m. (See Figure 6-26.) What fraction of the electrons in the beam will be transmitted through the barrier?

6-47. A beam of protons, each with kinetic energy 40 MeV, approaches a step potential of 30 MeV. (a) What fraction of the beam is reflected and transmitted? (b) How does your answer change if the particles are electrons?

### Level II

6-48. A proton is in an infinite square well potential given by Equation 6-21 with  $L = 1.0 \times 10^{-14}$  m. (a) Find the ground-state energy in MeV. (b) Make an energy-level diagram for this well. Calculate the wavelength of the photon emitted for the transitions (c)  $n = 2$  to  $n = 1$ , (d)  $n = 3$  to  $n = 2$ , and (e)  $n = 3$  to  $n = 1$ .

6-49. A particle is in the ground state of an infinite square well potential given by Equation 6-21. Calculate the probability that the particle will be found in the region (a)  $0 < x < \frac{1}{3}L$ , (b)  $0 < x < \frac{1}{3}L$ , and (c)  $0 < x < \frac{3}{4}L$ .

6-50. (a) Show that for large  $n$ , the fractional difference in energy between state  $n$  and state  $n + 1$  for a particle in an infinite square well is given approximately by

$$\frac{E_{n+1} - E_n}{E_n} \approx \frac{2}{n}$$

(b) What is the approximate percentage energy difference between the states  $n_1 = 1000$  and  $n_2 = 1001$ ? (c) Comment on how this result is related to Bohr's correspondence principle.

6-51. In this problem you will obtain the time-independent Schrödinger equation from the time-dependent equation by the method of separation of variables. (a) Substitute the trial function  $\Psi(x, t) = \psi(x)f(t)$  into Equation 6-6, and divide each term by  $\psi(x)f(t)$  to obtain the equation

$$i\hbar \frac{f'(t)}{f(t)} = -\frac{\hbar^2}{2m} \frac{\psi'(x)}{\psi(x)} + V(x)$$

(b) Since the left side of the equation in (a) does not vary with  $x$ , the right side cannot vary with  $x$ . Similarly, neither side can vary with  $t$ ; thus they both must equal some constant  $C$ . Show that this implies that  $f(t)$  is given by  $f(t) = e^{-i(C/\hbar)t}$ . Use the de Broglie relation to argue that  $C$  must be the total energy  $E$ . (c) Use the result of (b) to obtain Equation 6-14.

6-52. Quantum mechanics predicts that any particle localized in space has a nonzero velocity and consequently can never be at rest. Consider a Ping-Pong ball of diameter 2 cm and mass 2 g that can move back and forth in a box of length 2.001 cm. Hence, the space in which the ball moves is only 0.001 cm in length. (a) What is the minimum speed of the Ping-pong ball according to Schrödinger's equation? (b) What is the period of one oscillation?

6-53. A particle of mass  $m$  is in an infinite square well potential given by

$$\begin{aligned} V &= \infty & x < -\frac{1}{2}L \\ V &= 0 & -\frac{1}{2}L < x < +\frac{1}{2}L \\ V &= \infty & +\frac{1}{2}L < x \end{aligned}$$

Since this potential is symmetric about the origin, the probability density  $|\psi(x)|^2$  must also be symmetric. (a) Show that this implies that either  $\psi(-x) = \psi(x)$  or  $\psi(-x) = -\psi(x)$ . (b) Show that the proper solutions of the time-independent Schrödinger equation can be written

$$\psi(x) = \sqrt{\frac{2}{L}} \cos \frac{n\pi x}{L} \quad n = 1, 3, 5, 7, \dots$$

$$\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad n = 2, 4, 6, 8, \dots$$

Show that the allowed energies are the same as those for the infinite square well given in Equation 6-24.

6-54. The wave function  $\Psi_0(x) = Ae^{-x^2/2L^2}$  represents the ground-state energy of a harmonic oscillator. (a) Show that  $\psi_1 = L d\Psi_0(x)/dx$  is also a solution of Schrödinger's equation. (b) What is the energy of this new state? (c) From a look at the nodes of this wave function, how would you classify this excited state?

6-55. For the wave functions

$$\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad n = 1, 2, 3, \dots$$



corresponding to an infinite square well of length  $L$ , show that

$$\langle x^2 \rangle = \frac{L^2}{3} - \frac{L^2}{2n^2\pi^2}$$

**6-56.** A 10-eV electron is incident on a potential barrier of height 25 eV and width 1 nm. (a) Use Equation 6-76 to calculate the order of magnitude of the probability that the electron will tunnel through the barrier. (b) Repeat your calculation for a width of 0.1 nm.

**6-57.** A particle of mass  $m$  moves in a region in which the potential energy is constant  $V = V_0$ . (a) Show that neither  $\Psi(x, t) = A \sin(kx - \omega t)$  nor  $\Psi(x, t) = A \cos(kx - \omega t)$  satisfies the time-dependent Schrödinger equation. (Hint: If  $C_1 \sin \phi + C_2 \cos \phi = 0$  for all values of  $\phi$ , then  $C_1$  and  $C_2$  must be zero.) (b) Show that  $\Psi(x, t) = A[\cos(kx - \omega t) + i \sin(kx - \omega t)] = Ae^{i(kx - \omega t)}$  does satisfy the time-independent Schrödinger equation providing that  $k$ ,  $V_0$ , and  $\omega$  are related by Equation 6-5.

**6-58.** A particle of mass  $m$  on a table at  $z = 0$  can be described by the potential energy

$$V = mgz \quad \text{for } z > 0$$

$$V = \infty \quad \text{for } z < 0$$

For some positive value of total energy  $E$ , indicate the classically allowed region on a sketch of  $V(z)$  versus  $z$ . Sketch also the kinetic energy versus  $z$ . The Schrödinger equation for the problem is quite difficult to solve. Using arguments similar to those in Section 6-3 about the curvature of a wave function as given by the Schrödinger equation, sketch your "guesses" for the shape of the wave function for the ground state and the first two excited states.

### Level III

**6-59.** Use the Schrödinger equation to show that the expectation value of the kinetic energy of a particle is given by

$$\langle E_k \rangle = \int_{-\infty}^{+\infty} \psi(x) \left( -\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} \right) dx$$

**6-60.** An electron in an infinite square well with  $L = 10^{-12}$  m is moving at relativistic speed; hence, the momentum is *not* given by  $p = (2mE)^{1/2}$ . (a) Use the uncertainty principle to verify that the speed is relativistic. (b) Derive an expression for the electron's allowed energy levels and (c) compute  $E_1$ . (d) By what fraction does  $E_1$  computed in (c) differ from the nonrelativistic  $E_1$ ?

**6-61.** (a) Derive Equation 6-75. (b) Show that, if  $\alpha a \gg 1$ , Equation 6-76 follows Equation 6-75 as an approximation.

**6-62.** A beam of protons, each with energy  $E = 20$  MeV, is incident on a potential barrier 40 MeV high. Graph the relative probability of finding protons at values of  $x > 0$  from  $x = 0$  to  $x = 5$  fm. (Hint: Take  $|A|^2 = 1$  and refer to Example 6-6.)