Chapter 2

The Schrödinger Wave Equation

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The Schrödinger equation enables one to find the de Broglie wave associated with a particle and thus provides a basic tool for understanding microscopic phenomena.

The wave theory of matter originally proposed by de Broglie was further developed by Erwin Schrödinger who suggested that just as ray optics must be replaced by wave optics when light waves are obstructed by small objects, so classical mechanics must be replaced by wave mechanics in dealing with microscopic systems. Taking advantage of the analogy between optics and classical mechanics, Schrödinger obtained a differential equation which has come to be called the *Schrödinger equation*, and he used the equation to derive an expression for the energy levels of hydrogen obtaining results consistent with the earlier theory of Bohr. In this chapter, we shall obtain the Schrödinger equation and use this equation to study the properties of a number of physical problems in one dimension. Rather than following Schrödinger's original line of argument, we will show that the Schrödinger equation arises naturally in the context of the ideas of de Broglie and the results of electron diffraction experiments.

2.1 THE WAVE EQUATION

The electron diffraction experiments of Davisson and Germer and Thompson and Reid confirmed de Broglie's suggestion that a wave is associated with the motion of a particle. According to Eqs. (1.25) and (1.27), the momentum of the particle is related to the wavelength λ and angular wave vector k of the associated wave by the equations

$$p = \frac{h}{\lambda}, \tag{2.1}$$

and

$$p = \hbar k. \tag{2.2}$$

A relation between the kinetic energy of the particle and the angular wave vector can be obtained by writing the kinetic energy in terms of the momentum as follows

$$KE = \frac{1}{2}mv^2 = \frac{1}{2m}(mv)^2.$$

This last equation can be written

$$KE = \frac{1}{2m}p^2, \tag{2.3}$$

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where p is the momentum of the particle. Substituting Eq. (2.2) into Eq. (2.3) gives

$$KE = \frac{(\hbar k)^2}{2m}.$$

The form of the wave function for a stationary wave is given by Eq. (I.23) of the introduction. We have

$$\psi(x) = A\mathrm{e}^{\mathrm{i}kx}. \tag{2.4}$$

Following de Broglie, we shall suppose that the wave function (2.4) is associated with the motion of a free particle and refer to this function simply as the de Broglie wave function. For a free particle, the potential energy is constant and may be taken to be zero. The energy of the particle is then

$$E = \frac{(\hbar k)^2}{2m}. \tag{2.5}$$

The Davisson-Germer diraction experiments can be successfully explained by associating a de Brogllie wave function with the beam of freely moving electrons. For the de Broglie wave function (2.4) with the angular wave vector k, the particles associated with the wave have momentum and energy given by Eqs. (2.2) and (2.5). Equations (2.2), (2.4), and (2.5) together provide a concise summary of the experimental results.

We shall now find differential equations that are satisfied by the de Broglie function (2.4). Taking the derivative of Eq. (2.4) with respect to x, we obtain

$$\frac{\mathrm{d}\psi}{\mathrm{d}x} = Aik\mathrm{e}^{\mathrm{i}kx} = \mathrm{i}k\psi.$$

We can simplify this result by multiplying the equation through from the left with $-\mathrm{i}\hbar$ to get

$$-\mathrm{i}\hbar\frac{\mathrm{d}\psi}{\mathrm{d}x} = \hbar k\psi,$$

and then using Eq. (2.2) to identify the term $\hbar k$ appearing on the right as the momentum p. The differential equation satisfied by the de Broglie wave function (2.4) can thus be written as

$$-\mathrm{i}\hbar\frac{\mathrm{d}\psi}{\mathrm{d}x} = p\psi. \tag{2.6}$$

Another equation satisfied by the de Broglie wave function can be obtained by taking the derivative of Eq. (2.6) with respect to x and then multiplying the resulting equation through by $-\mathrm{i}\hbar$. We get

$$-\hbar^2\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -\mathrm{i}p\hbar\frac{\mathrm{d}\psi}{\mathrm{d}x}.$$

This equation can be simplified using Eq. (2.6) to evaluate the term on the right giving

$$-\hbar^2\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = p^2\psi.$$

We then divide the equation through by $2m$ and use the relation, $E = p^2/2m$, to replace the coefficient of the wave function on the right by the energy

$$\frac{-\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi. \tag{2.7}$$

Since the de Broglie function $\psi(x) = A\mathrm{e}^{\mathrm{i}kx}$ is a solution of Eq. (2.7) with $E = \hbar^2k^2/2m$, this equation may be thought of as the equation associated with a free particle with energy E.

To obtain a general equation that would apply to any particle with potential energy $V(x)$, we first note that Eq. (2.7) was obtained by taking the second derivative of the de Broglie wave function (2.4) which is known to describe a free particle. Substituting Eq. (2.4) into Eq. (2.7) gives

$$\frac{\hbar^2k^2}{2m}A\mathrm{e}^{\mathrm{i}kx} = EA\mathrm{e}^{\mathrm{i}kx}.$$

Notice that the coefficient of the de Broglie wave function on the left-hand side of this equation is the kinetic energy of the particle. An obvious way of extending Eq. (2.7) to include the effects of an external force is to add a second term to the left-hand side of Eq. (2.7) corresponding to the potential energy of the particle. We thus write

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi. \tag{2.8}$$

This equation, which was originally obtained by Schrödinger in 1926, is called the *Schrödinger time-independent equation*. The Schrödinger equation (2.8) reduces to the free-particle equation (2.7) when the potential energy is equal to zero.

We shall presently solve the Schrödinger equation (2.8) for a number of different physical problems and find that the equation provides a convincing description of microscopic systems. The validity of the Schrödinger equation depends ultimately upon how well the predictions of the theory are confirmed by experiments.

The theory of Schrödinger provides a means for studying the de Broglie waves, which can be thought of as solutions of the Schrödinger equation. The Schrödinger equation also gives the correct energy levels of hydrogen, and thus provides a framework for understanding the earlier results of Balmer and Bohr. When Schrödinger first presented his theory, though, he was unsure how the wave function should be interpreted. To overcome this difficulty, Max Born, who made numerous contributions to the new quantum theory, proposed an interpretation of the wave function in terms of probabilities. Born suggested that the probability of finding the particle in a particular location depended upon the absolute value squared of the wave function. More precisely, the probability dP that the particle is in the infinitesimal interval between x and $x + dx$ is given by the equation

$$dP = |\psi(x)|^2\, dx, \tag{2.9}$$

where $|\psi(x)|^2$ is the product of the function $\psi(x)$ and its complex conjugate $\psi^*(x)$

$$|\psi(x)|^2 = \psi^*(x)\psi(x).$$

Equation (2.9), which defines the relation between the probability and the wave function, can also be written

$$|\psi(x)|^2 = \frac{dP}{dx},$$

and we may thus refer to $|\psi(x)|^2$ as the *probability density*.

The wave mechanical theory of Schrödinger with the probabilistic interpretation of Born is now widely accepted as providing an accurate description of microscopic systems. In this chapter, we shall use this theory to study the properties of a number of physical problems in one dimension.

Example 2.1

Find the wave function and the energy levels of a particle that is confined within the infinite potential well shown in Fig. 2.1.

Solution

The potential energy function $V(x)$ shown in Fig. 2.1 is equal to zero within the well. Substituting $V(x) = 0$ in Eq. (2.8), we obtain the equation,

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi, \tag{2.10}$$

for the wave function $\psi(x)$ within the well with x is in the range $-L/2 \le x \le +L/2$. The probability of finding the particle at a particular point may be obtained from the wave function using Eq. (2.9). Since the particle is confined within the interior of the potential well, the wave function is zero beyond the well boundaries at $x = \pm L/2$.

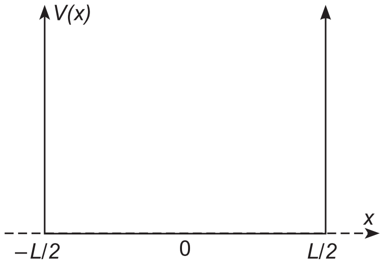

FIGURE 2.1 An infinite potential well extending from $x = -L/2$ to $x = L/2$.

A careful analysis shows that the wave function and its derivative must be continuous at the boundaries of the well. Here, we only give the reason in general terms. We will find that in addition to a probability density one can also define a current density which describes the flow of particles within the well. If the wave function or its derivative were discontinuous at $x = \pm L/2$, the boundaries of the well would serve as an emitter or an absorber of particles. This would violate the demonstrable properties of the probability and current densities which together satisfy the requirement that the flow of probability into a region is equal to the rate that the probability the particle is in the region increases.

Since the wave function, $\psi(x)$, is continuous and is equal to zero within the walls of the well, the wave function must approach zero as x approaches $-L/2$ or $+L/2$. We thus require that the solutions of Eq. (2.10) satisfy the following boundary conditions

$$\begin{aligned} \psi(-L/2) &= 0, \\ \psi(+L/2) &= 0. \end{aligned} \tag{2.11}$$

In order to be in a better position to solve the Schrödinger equation (2.10), we bring the term $E\psi$ over to the left-hand side of the equation, and then multiply the entire equation through by $-2m/\hbar^2$ to obtain

$$\frac{d^2\psi}{dx^2} + \left(\frac{2mE}{\hbar^2}\right)\psi = 0.$$

Defining

$$k^2 = \left(\frac{2mE}{\hbar^2}\right), \tag{2.12}$$

the Schrödinger equation becomes

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0. \tag{2.13}$$

One may readily confirm that the functions,

$$\psi(x) = A\cos(kx)$$

and

$$\psi(x) = B\sin(kx),$$

are solutions of Eq. (2.13). For instance, substituting $\psi(x) = A\cos(kx)$ into Eq. (2.13) gives

$$\frac{d^2\left(A\cos(kx)\right)}{dx^2} + k^2A\cos(kx) = -Ak^2cos(kx) + k^2A\cos(kx) = 0.$$

The cosine function is an even function of x being unchanged when x is replaced by $-x$, while the sine function is an odd function of x changing its sign when x is replaced by $-x$.

First, we consider the even solutions. Inside the well, the even solutions have the form

$$\psi(x) = A\cos kx, \quad \text{for } -L/2 \le x \le L/2. \tag{2.14}$$

These solutions satisfy the boundary conditions (2.11) provided that

$$kL/2 = n\pi/2,$$

where n is an odd integer. Similarly, the odd functions,

$$\psi(x) = A\sin kx, \quad \text{for } -L/2 \le x \le L/2, \tag{2.15}$$

satisfy the boundary conditions (2.11) provided that

$$kL/2 = n\pi/2,$$

where n is an even integer. The conditions imposed upon the even and odd solutions both lead to the equation

$$k = \frac{n\pi}{L}, \tag{2.16}$$

where the integer n may be odd or even.

The even solution corresponding $n = 1$ is

$$\psi(x) = A\cos\left(\frac{\pi x}{L}\right),$$

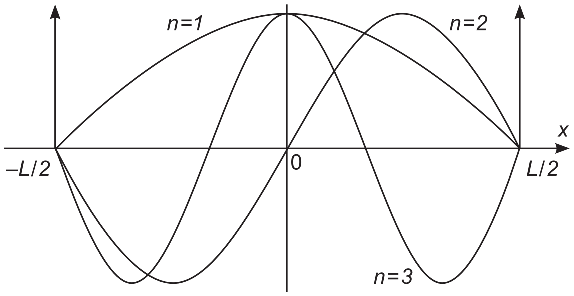

FIGURE 2.2 The solutions of the Schrödinger equation for the infinite well for n =1,2, and 3. Solutions with n odd are even and solutions with n even are odd.

while the odd solution corresponding to $n = 2$ is

$$\psi(x) = A \sin\left(\frac{2\pi x}{L}\right).$$

One can readily confirm that the solutions of the Schrödinger equation for $n = 1$ and $n = 2$ go to zero on the boundary. For larger values of n, the solutions with n odd are even, and solutions with n even are odd. Figure 2.2 shows the solutions of the Schrödinger equation for the infinite well corresponding to $n = 1, 2,$ and 3.

Solving Eq. (2.12) for the energy, we obtain

$$E = \frac{\hbar^2 k^2}{2m}.$$

An equation for the energy in terms of the integer n can then be obtained by substituting Eq. (2.16) into the above equation giving

$$E = \frac{n^2\pi^2\hbar^2}{2mL^2}.$$

Using the fact that $\hbar = h/2\pi$, this last equation may be written more simply

$$E = \frac{n^2h^2}{8mL^2}. \tag{2.17}$$

The wave functions and the values of the energy of a particle moving in an infinite well depend upon the positive integer n, which is called a *quantum number*.

The wave functions shown in Fig. 2.2 have the form of standing waves. As for the functions describing the displacement of a guitar string, the wave function of a particle in an infinite well is equal to zero at the ends of the physical region. The displacement of a guitar string must be zero at the ends because the string is tied, while the wave function of a particle in an infinite well must be zero because the particle cannot penetrate the infinite walls of the well.

2.2 PROBABILITIES AND AVERAGE VALUES

The probability dP of finding the particle at a particular point in space is related to the absolute value squared of the wave function. According to Eq. (2.9), the probability that the particle is in the infinitesimal interval between x and $x + \mathrm{d}x$ is equal to

$$\mathrm{d}P = |\psi(x)|^2 \,\mathrm{d}x.$$

The probability of finding the particle between two points, x_1 and x_2, may be obtained by integrating this last equation for dP over the range between x_1 and x_2. We have

$$P(x_1 \to x_2) = \int_{x_1}^{x_2} |\psi(x)|^2 \,\mathrm{d}x.$$

In performing the above integration, one adds up the probabilities for the infinitesimal intervals between x_1 and x_2. The requirement that the total probability of finding the particle at any point along the x-axis is equal to one can be written

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1, \tag{2.18}$$

where the integration is performed over the entire range of the variable x. The condition (2.18) is referred to as the *normalization condition*. It enables us to calculate the value of the constant A in the previous example.

Example 2.2

Use the normalization condition to evaluate the constant A for the wave functions in Example 2.1.

Solution

Since the particle in the infinite well shown in Fig. 2.1 must be located between $-L/2$ and $+L/2$, the probability of finding the particle in the range between $-L/2$ and $+L/2$ must be equal to one. We have

$$\int_{-L/2}^{L/2} |\psi(x)|^2 \mathrm{d}x = 1. \tag{2.19}$$

The even solutions for the particle in the infinite well can be obtained using Eqs. (2.14) and (2.16). We obtain

$$\psi(x) = A\cos\left(\frac{n\pi x}{L}\right).$$

Substituting this wave function into the integral in Eq. (2.19) gives

$$A^2 \int_{-L/2}^{L/2} \cos^2\left(\frac{n\pi x}{L}\right) \mathrm{d}x = 1.$$

In order to evaluate the above definite integral, we first note that the integral gives the area under the curve of the function $\cos^2(n\pi x/L)$ for a number of half periods. This area is the same as the area under the curve of the function $\sin^2(n\pi x/L)$. We may thus replace $\cos^2(n\pi x/L)$ with $\frac{1}{2}[\sin^2(n\pi x/L) + cos^2(n\pi x/L)]$ in the above integral to obtain

$$A^2 \int_{-L/2}^{L/2} \frac{1}{2}\left[\sin^2\left(\frac{n\pi x}{L}\right) + \cos^2\left(\frac{n\pi x}{L}\right)\right] \mathrm{d}x = 1.$$

Using the identity, $\sin^2(n\pi x/L) + \cos^2(n\pi x/L) = 1$, the last equation may be written simply

$$A^2 \int_{-L/2}^{L/2} \frac{1}{2} \mathrm{d}x = 1.$$

Since the above integral has the value $L/2$, we obtain the result

$$A = \sqrt{\frac{2}{L}}.$$

The normalization constant A for the odd functions can be shown to be given by the same equation.

Using this result, the wave function of a particle in an infinite well can be written

$$\psi_n(x) = \begin{cases} \sqrt{2/L}\cos(n\pi x/L), & n \text{ odd} \\ \sqrt{2/L}\sin(n\pi x/L). & n \text{ even} \end{cases} \tag{2.20}$$

The absolute value of the wave function squared gives the probability density of finding the particle at a particular point along the x-axis. For most problems, the probability density will be non-zero over a range of values of x, and a measurement of x may lead to any value within the range. We can still use the wave function, though, to predict the average value of a large number of different measurements of x. In order to motivate the formula that we shall use for the average value of an observable, we consider the problem of determining the average age of the students in a class. Suppose that there are n_1 students having an age a_1, n_2 students having an age a_2, and so forth, and suppose that the total number of students is N. Then the average age of the students in the class will be

$$\text{Average age} = \frac{\sum_i a_i n_i}{N},$$

where the sum runs over all of the different possible ages of the students. This last equation can be written

$$\text{Average age} = \sum_i a_i \left(\frac{n_i}{N}\right),$$

where N has been brought inside the summation. For each value of i, the ratio n_i/N is equal to the probability P_i of a student having the age a_i. So this last result can be written

$$\text{Average age} = \sum_i a_i P_i.$$

In exactly the same way, the average position of a particle can be calculated using the equation

$$\langle x \rangle = \int_{-\infty}^{\infty} x|\psi(x)|^2 \, \mathrm{d}x, \tag{2.21}$$

where the integration is extended over the entire range of the variable x. The above integration adds up the contributions from all the infinitesimal intervals from $-\infty$ to ∞. For each interval, x is multiplied by the probability that a particle should be in the infinitesimal interval containing x. This formula for calculating the average value of x may be extended so that it enables us to calculate the average value of an arbitrary function of x

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} f(x)|\psi(x)|^2 \, \mathrm{d}x.$$

We now give the following example of the application of this formula.

Example 2.3

A particle, which is confined to move in one dimension between 0 and L, is described by the wave function

$$\psi(x) = A\,x(L - x). \tag{2.22}$$

Use the normalization condition (2.18) to determine the constant A and then derive an expression for the average value of the position of the particle.

Solution

Since the particle is located between 0 and L, the normalization condition is

$$\int_0^L |\psi(x)|^2 \, \mathrm{d}x = 1.$$

Substituting the wave function (2.22) into this equation, we get

$$A^2 \int_0^L x^2(L - x)^2 \, \mathrm{d}x = 1.$$

To evaluate the above integral we multiply the terms in the integrand together to obtain

$$A^2 \int_0^L (L^2 x^2 - 2L x^3 + x^4) \, \mathrm{d}x = 1,$$

and then integrate the polynomial in the integrand term for term to get

$$A^2 \left[\frac{L^2 x^3}{3} - \frac{2Lx^4}{4} + \frac{x^5}{5} \right]_0^L = 1.$$

The left-hand side of the above equation is evaluated by first substituting $x = L$ into the expression within square brackets and then subtracting the result obtained by substituting $x = 0$ into the expression. We notice that all of the terms obtained by substituting $x = L$ contain a factor of L^5 and all the terms obtained by substituting $x = 0$ give zero. The above equation thus becomes

$$A^2 L^5 \left[\frac{1}{3} - \frac{1}{2} + \frac{1}{5} \right] = A^2 L^5 \frac{1}{30} = 1.$$

Solving for A, we obtain

$$A = \sqrt{\frac{30}{L^5}}.$$

and the wave function can be written

$$\psi(x) = \sqrt{\frac{30}{L^5}}\, x(L - x). \tag{2.23}$$

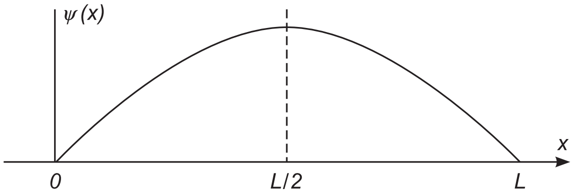

FIGURE 2.3 The function $\psi(x) = Ax(L-x)$, for x in the range, $0 \le x \le L$.

In order to obtain the average value of the position, we substitute the wave function (2.23) into Eq. (2.21) to obtain

$$\langle x\rangle = \int_0^L x\,\frac{30}{L^5}\,x^2(L-x)^2\,dx = \frac{30}{L^5}\int_0^L (L^2x^3 - 2Lx^4 + x^5)\,dx.$$

Evaluating the last integral, we obtain

$$\langle x\rangle = \frac{30}{L^5}\left[\frac{L^2x^4}{4} - \frac{2Lx^5}{5} + \frac{x^6}{6}\right]_0^L.$$

At this point, we note again that all terms obtained by substituting $x = L$ into the expression within square brackets contain a factor of L^6 and all the terms obtained by substituting $x = 0$ give zero. We thus obtain

$$\langle x\rangle = \frac{30L^6}{L^5}\left[\frac{1}{4} - \frac{2}{5} + \frac{1}{6}\right] = \frac{L}{2}.$$

Notice that the wave function shown in Fig. 2.3 is symmetric with respect to the dotted vertical line passing through the maximum of the function at $x = L/2$ and that the average value of x corresponds to the value of x for which the function attains its maximum. One must be aware, though, that the average value of x does not generally coincide with the maximum value of the wave function.

2.3 THE FINITE POTENTIAL WELL

The infinite potential well provides a simple application of the ideas of quantum theory leading to simple formulas for the energy levels and wave functions of particles. Because the model is so simple and because a particle in an infinite well has discrete energy levels, the infinite well is still widely used. The finite potential well shown in Fig. 2.4 also has discrete energy levels and provides a more realistic description of a number of important physical systems. As we shall see, the finite potential well gives a realistic description of the environment of electrons trapped within the layers of semiconductors and the environment of protons and neutrons in an atomic nucleus.

The approach we shall use for the finite well is more complex than the approach we adopted for the infinite well. For the infinite well, we solved the Schrödinger equations inside the well and then required that the wave functions go to zero on the boundary. In contrast, we shall now solve the Schrödinger equation corresponding to the finite well for values of x inside

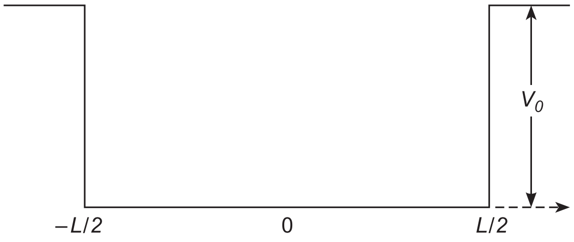

FIGURE 2.4 A finite well of depth V_0 extending from $x = -L/2$ to $x = L/2$.

and outside the well, and we shall then match the solutions in these regions at the boundary. As for the infinite potential well, the Schrödinger equation inside the finite well is

$$\frac{-\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi, \quad \text{for } -L/2 \leq x \leq L/2. \tag{2.24}$$

This equation can be written

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + k^2\psi = 0, \tag{2.25}$$

where

$$k = \left(\frac{2mE}{\hbar^2}\right)^{1/2}. \tag{2.26}$$

The finite well shown in Fig. 2.4 has a depth V_0. Outside the well, the Schrödinger equation is

$$\frac{-\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V_0\psi = E\psi, \quad \text{for } |x| \geq L/2. \tag{2.27}$$

For values of the energy E less than the well depth V_0, the Schrödinger equation for the region outside the well can be written

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} - \kappa^2\psi = 0, \tag{2.28}$$

where

$$\kappa = \left[\frac{2m(V_0 - E)}{\hbar^2}\right]^{1/2}. \tag{2.29}$$

Notice that E being less than V_0 implies that $V_0 - E$ is positive and that κ is a real number.

There are even and odd solutions of the Schrödinger equation inside the finite well—just as there are for the infinite well. Each solution of the Schrödinger equation inside the finite well can be joined with a solution of the Schrödinger equation outside the well. We consider first the even bound solutions. Inside the well, the even solutions are

$$\psi(x) = A\cos kx, \quad \text{for } -L/2 \leq x \leq L/2. \tag{2.30}$$

We can concentrate on the portion of the solution outside the well for $x > L/2$ and obtain the solution for $x < -L/2$ from symmetry. For $x > L/2$, the solution of Eq. (2.28) can be written

$$\psi(x) = B\exp(-\kappa x), \quad \text{for } x \geq L/2, \tag{2.31}$$

where we have taken the negative sign in the above exponent so that the wave function decreases to zero for large distances and is hence normalizable.

We now require that the solution be continuous at $x = L/2$ and obtain

$$A\cos(kL/2) = B\exp(-\kappa L/2). \tag{2.32}$$

Similarly, the condition that the derivative of the solution be continuous at $x = L/2$ leads to the equation

$$-Ak\sin(kL/2) = -B\kappa\exp(-\kappa L/2). \tag{2.33}$$

We can eliminate the constants, A and B, from the last two equations by dividing Eq. (2.33) by Eq. (2.32) giving

$$\tan(kL/2) = \frac{\kappa}{k}.$$

While the above equation cannot be solved exactly, it can be transformed into a form suitable for obtaining a numerical solution. Substituting Eq. (2.29) into this last equation, we get

$$\tan(kL/2) = \sqrt{\frac{2mV_0}{\hbar^2k^2} - \frac{2mE}{\hbar^2k^2}}.$$

We may now use Eq. (2.26) to simplify the second term within the square root of the above equation to obtain

$$\tan(kL/2) = \sqrt{\frac{2mV_0}{\hbar^2k^2} - 1}.$$

This last equation can be expressed as follows in terms of the dimensionless variable

$$\theta = kL/2. \tag{2.34}$$

We have

$$\tan\theta = \sqrt{\frac{\theta_0^2}{\theta^2} - 1}, \tag{2.35}$$

where

$$\theta_0^2 = \frac{mV_0L^2}{2\hbar^2}. \tag{2.36}$$

Thus far, we have only considered the even solutions of the Schrödinger equation. Inside the well, the odd solutions are

$$\psi(x) = A\sin kx, \quad \text{for } -L/2 \le x \le L/2. \tag{2.37}$$

Imposing the boundary conditions at $x = L/2$ as before leads to the equation

$$-\cot\theta = \sqrt{\frac{\theta_0^2}{\theta^2} - 1}, \tag{2.38}$$

where the variable θ is again equal to $kL/2$ and θ_0 is given by Eq. (2.36). The energies for the bound solutions may be obtained by plotting the left- and right-hand sides of Eqs. (2.35) and (2.38) and noting where the curves cross.

The solutions of the Schrödinger equation with energy E greater than V_0 are considered in Problem 10. Solutions of the Schrödinger equation can be found for all values of the energy greater than the well depth V_0. The wave functions for $E > V_0$ are oscillatory functions called *continuum states*, while the wave functions for $E < V_0$, which are confined to the vicinity of the well, are called *bound states*.

As a first example of a finite well, we consider a structure that is formed with layers of the semiconductors, GaAs, and AlGaAs. GaAs is a semiconductor with Ga at one set of sites in the crystal and As at the other sites. Crystals composed of the alloy, $Al_xGa_{1-x}As$ have Al or Ga at one set of sites in the crystal and As at the other sites. The indices, x and $1 - x$, give the fractional number of the corresponding species in the crystal. As will be discussed in Chapter 10, the alloys of gallium arsenide GaAs and indium phosphide InP are useful for making light-emitting diodes and semiconductor lasers because the conduction electrons of these compounds can make direct optical transitions to unoccupied states in the lower-lying valence shell.

Figure 2.5 shows the energies available to conduction electrons for a structure in which one layer of GaAs is sandwiched between two layers of $Al_{0.3}Ga_{0.7}As$. The $Al_{0.3}Ga_{0.7}As$ crystal has 30% aluminum and 70% gallium. The range of energies available to conduction electrons in GaAs in the center dips down below the levels of $Al_{0.3}Ga_{0.7}As$ on the two sides. Electrons near the bottom of the conduction band of GaAs are not free to move because there are no available states of the same energy in $Al_{0.3}Ga_{0.7}As$. This situation is generally described by saying that the conduction electrons in GaAs are confined within a *quantum well*. As can be seen in Fig. 2.5, the depth of the quantum well created with GaAs sandwiched between two layers of $Al_{0.3}Ga_{0.7}As$ is about 0.3 eV.

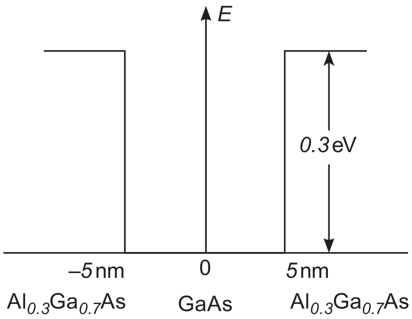

FIGURE 2.5 Energies of conduction electron for a structure in which one layer of GaAs is sandwiched between two layers of $Al_{0.3}Ga_{0.7}As$. Electrons in GaAs are in a quantum well of depth 0.30 eV and width 10 nm.

The periodic potential due to the atoms in a crystal can enhance or retard the motion of the conduction electrons. As will be discussed in Chapter 9, the screening of the charge of conduction electrons by the ions of the crystal can cause the effective mass of the electrons in a crystal to differ considerably from the mass of free electrons. The effective mass of conduction electrons in GaAs is equal to 0.067 times the free electron mass. Using this value of the mass of the electron, the value of θ_0^2 for an electron confined to a quantum well with a depth of 0.3 eV and thickness of $L = 10$ nm in GaAs is found to be 13.2. This value of θ_0 can be substituted into the right-hand side of Eq. (2.35) and the left- and right-hand sides of the equation plotted to find the points where the curves corresponding to the two sides of the equation intersect. A MATLAB program for determining the points of intersections for left- and right-hand sides of Eqs. (2.35) and (2.38) is given in the following MATLAB program.

MATLAB Program 2.1

This program determines the points of intersections for left- and right-hand side of Eq. (2.35) and (2.38).

```
theta0 = sqrt(13.2);
theta = linspace(0.275, theta0,400);
y = sqrt(theta0^2 ./ theta.^2-1.0);
theta1 = linspace(0.0,0.5*pi-0.075,400);
y1 = tan(theta1);
theta2 = linspace(0.5*pi,pi-0.075,400);
y2 = -cot(theta2);
theta3 = linspace(pi,1.5*pi-0.075,400);
y3 = tan(theta3);
plot(theta,y, theta1,y1, theta2,y2, theta3,y3)
```

Before plotting the left- and right-hand sides of Eqs. (2.35) and (2.38), we first note that the common right-hand side of the two equations becomes become infinite at $\theta = 0$ and assumes imaginary values for θ greater than $\theta_0 = 3.63$. The right-hand side of the equations can be plotted from a value slightly greater than zero to θ_0. In contrast, the left-hand sides of Eqs. (2.35) and (2.38) must be plotted in segments because $\tan(\theta)$ become infinite at $\pi/2$ and $3\pi/2$, while $\cot(\theta)$ becomes infinite at π. The first line of the MATLAB Program 2.1 defines the value of θ_0. As described in Appendix C, the second line of the program then produces a vector, theta, consisting of values of θ for 400 equally-spaced points between 0.275 and θ_0. The next line of code produces a vector, y, having the values of the common right-hand side of Eqs. (2.35) and (2.38) at the points theta. The fourth line of the program produces a vector, theta1, with value of θ from 0.0 to a point slightly before $\pi/2$ where the tangent function is singular, and the next line defines a vector, y1, giving the values of the tangent at those values of θ. Similarly, theta2 is a vector with the value of θ between $\pi/2$ and slightly before π, and theta3 is a vector with the values of θ between π and slightly before $3\pi/2$. y2 gives the value of the negative of the cotangent for the points theta2, and y3 gives the value of the tangent for the points theta3. The last line of the program produces the plot shown in Fig. 2.6(a). The energy of the even solutions correspond to the points where the tangent curve intersects the curve corresponding to the right-hand side of the equations, while the energy of the odd solutions correspond to the point where

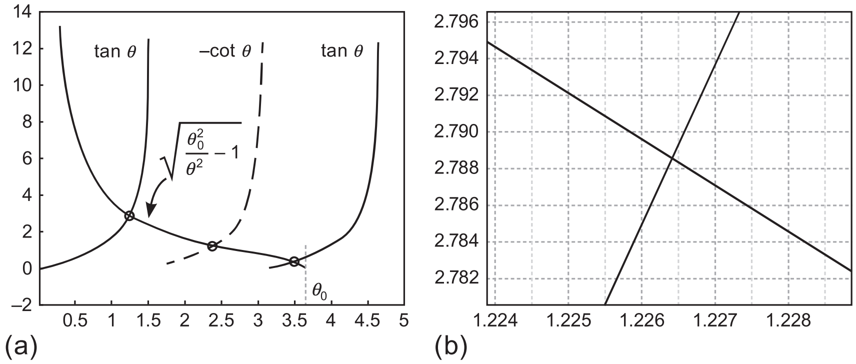

FIGURE 2.6 (a) Graphical solution of Eqs. (2.35) and (2.38) for a quantum well for which $\theta_0^2 = 13.2$. The well has three bound states. (b) The figure used to estimated the value of θ for the first intersection of the curves shown in Fig. 2.6(a).

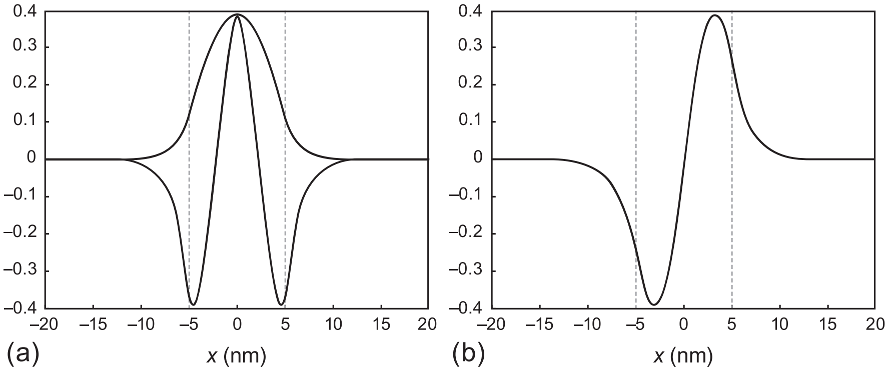

FIGURE 2.7 (a) The even bound solutions of an electron in a finite well. (b) The odd bound solution of an electron in a finite well.

the negative of the cotangent intersects the curve corresponding to the right-hand side MATLAB Program 2.1 also runs on the free software package Octave producing a figure very similar to Fig. 2.6(a).

An accurate estimate of the value of θ where the curve of the tangent function between zero and $\pi/2$ intersects the curve corresponding to the right-hand side can be obtained by clicking on the icon looking like a magnifying glass with a plus sign in the middle, bringing it down to the point where the two curves intersect, and clicking several times on the point of intersection. Issuing the MATLAB command `grid on` then produces Fig. 2.6(b). In this way, we estimated the value of θ for the first intersection to be 1.2264. The value of the energy for a particular value of θ can be calculated by using the definition, $\theta = kL/2$ and Eq. (2.26) to derive the equation

$$E = \frac{2\hbar^2\theta^2}{mL^2}. \tag{2.39}$$

Substituting $\theta = 1.2264$ into this equation gives $E = 0.0342$ eV. We shall denote the energy of the lowest stately by E_1 and the wave function of the lowest state by ψ_1. Similarly, we found the values of θ for the other two points of intersection to be 2.4347 and 3.4556 corresponding to the energies $E_2 = 0.1326$ eV and $E_3 = 0.2714$. The wave functions for these two states will be denoted by ψ_2 and ψ_3 respectively. The energy E_3 corresponds to a very loosely bound electron with an energy near the top of the well.

For a particular value of θ, the values of k and κ are given by the equations

$$k = \frac{2\theta}{L}, \tag{2.40}$$

$$\frac{\kappa}{k} = \sqrt{\frac{\theta_0^2}{\theta^2} - 1}, \tag{2.41}$$

The first of these two equations follows immediately from the definition of θ given by Eq. (2.34). A derivation of the second equation is left as an exercise (see Problem 11). Using MATLAB and the values of θ determine graphically together with Eqs. (2.30), (2.31), and (2.37), we plotted the even functions obtaining the functions shown in Fig. 2.7(a) and the odd function shown in Fig. 2.7(b).

Our second illustration of finite potential wells is taken from nuclear physics. Figure 2.8 shows the lowest single-nucleon states of the $^{15}_{8}$O and $^{17}_{8}$O nuclei. The $^{15}_{8}$O nucleus has eight protons and seven neutrons, while the $^{17}_{8}$O nucleus has eight protons and nine neutrons. As discussed in Chapter 13, the properties of the ground states of each of these nuclei are due to the unpaired neutron.

2.4 THE SIMPLE HARMONIC OSCILLATOR

Another important problem that can be treated readily using the wave mechanical ideas we have introduced in this chapter is the simple harmonic oscillator illustrated in Fig. I.2. The classical oscillator consists of a particle of mass m moving under