Chapter 4

One-Dimensional Problems

4.1 Introduction

After presenting the formalism of quantum mechanics in the previous two chapters, we are now well equipped to apply it to the study of physical problems. Here we apply the Schrödinger equation to *one-dimensional* problems. These problems are interesting since there exist many physical phenomena whose motion is one-dimensional. The application of the Schrödinger equation to *one-dimensional* problems enables us to compare the predictions of classical and quantum mechanics in a simple setting. In addition to being simple to solve, one-dimensional problems will be used to illustrate some nonclassical effects.

The Schrödinger equation describing the dynamics of a microscopic particle of mass m in a one-dimensional time-independent potential $V(x)$ is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x), \tag{4.1}$$

where E is the total energy of the particle. The solutions of this equation yield the allowed energy eigenvalues E_n and the corresponding wave functions $\psi_n(x)$. To solve this partial differential equation, we need to specify the potential $V(x)$ as well as the boundary conditions; the boundary conditions can be obtained from the physical requirements of the system.

We have seen in the previous chapter that the solutions of the Schrödinger equation for time-independent potentials are stationary,

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}, \tag{4.2}$$

for the probability density does not depend on time. Recall that the state $\psi(x)$ has the physical dimensions of $1/\sqrt{L}$, where L is a length. Hence, the physical dimension of $|\psi(x)|^2$ is $1/L$: $\left[|\psi(x)|^2\right] = 1/L$.

We begin by examining some general properties of one-dimensional motion and discussing the symmetry character of the solutions. Then, in the rest of the chapter, we apply the Schrödinger equation to various one-dimensional potentials: the free particle, the potential step, the finite and infinite potential wells, and the harmonic oscillator. We conclude by showing how to solve the Schrödinger equation numerically.

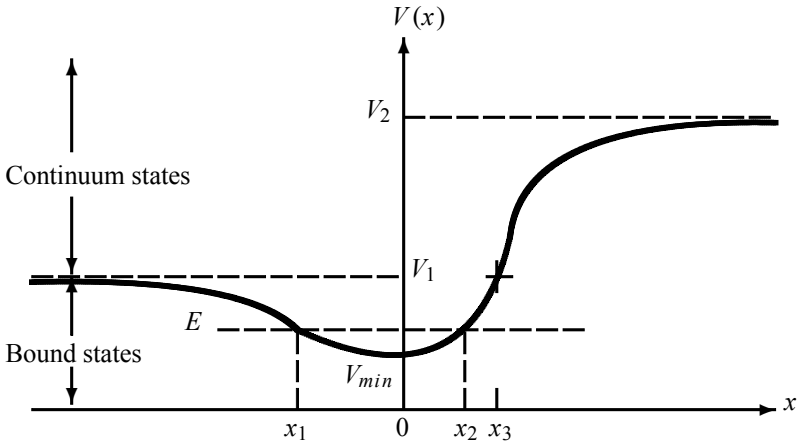


Figure 4.1 Shape of a general potential.

4.2 Properties of One-Dimensional Motion

To study the dynamic properties of a single particle moving in a one-dimensional potential, let us consider a potential $V(x)$ that is general enough to allow for the illustration of all the desired features. One such potential is displayed in Figure 4.1; it is finite at $x \to \pm\infty$, $V(-\infty) = V_1$ and $V(+\infty) = V_2$ with V_1 smaller than V_2, and it has a minimum, V_{min}. In particular, we want to study the conditions under which discrete and continuous spectra occur. As the character of the states is completely determined by the size of the system's energy, we will be considering separately the cases where the energy is smaller and larger than the potential.

4.2.1 Discrete Spectrum (Bound States)

Bound states occur whenever the particle cannot move to infinity. That is, the particle is *confined* or *bound* at all energies to move within a *finite* and limited region of space which is delimited by two classical turning points. The Schrödinger equation in this region admits only solutions that are *discrete*. The infinite square well potential and the harmonic oscillator are typical examples that display bound states.

In the potential of Figure 4.1, the motion of the particle is bounded between the classical turning points x_1 and x_2 when the particle's energy lies between V_{min} and V_1:

$$V_{min} < E < V_1. \tag{4.3}$$

The states corresponding to this energy range are called *bound* states. They are defined as states whose wave functions are finite (or zero) at $x \to \pm\infty$; usually the bound states have energies smaller than the potential $E < V$. For the bound states to exist, the potential $V(x)$ must have at least one minimum which is lower than V_1 (i.e., $V_{min} < V_1$). The energy spectra of bound states are discrete. We need to use the boundary conditions[1] to find the wave function and the energy.

Let us now list two theorems that are important to the study of bound states.

[1] Since the Schrödinger equation is a *second-order* differential equation, only *two* boundary conditions are required to solve it.

Theorem 4.1 *In a one-dimensional problem the energy levels of a bound state system are discrete and not degenerate.*

Theorem 4.2 *The wave function $\psi_n(x)$ of a one-dimensional bound state system has n nodes (i.e., $\psi_n(x)$ vanishes n times) if $n = 0$ corresponds to the ground state and $(n-1)$ nodes if $n = 1$ corresponds to the ground state.*

4.2.2 Continuous Spectrum (Unbound States)

Unbound states occur in those cases where the motion of the system is not confined; a typical example is the *free* particle. For the potential displayed in Figure 4.1 there are two energy ranges where the particle's motion is infinite: $V_1 < E < V_2$ and $E > V_2$.

- Case $V_1 < E < V_2$

  In this case the particle's motion is infinite only towards $x = -\infty$; that is, the particle can move between $x = x_3$ and $x \to -\infty$, x_3 being a classical turning point. The energy spectrum is continuous and none of the energy eigenvalues is degenerate. The nondegeneracy can be shown to result as follows. Since the Schrödinger equation (4.1) is a second-order differential equation, it has, for this case, two linearly independent solutions, but only one is physically acceptable. The solution is oscillatory for $x \leq x_3$ and rapidly decaying for $x > x_3$ so that it is finite (zero) at $x \to +\infty$, since divergent solutions are unphysical.

- Case $E > V_2$

  The energy spectrum is continuous and the particle's motion is infinite in both directions of x (i.e., towards $x \to \pm\infty$). All the energy levels of this spectrum are doubly degenerate. To see this, note that the general solution to (4.1) is a linear combination of two independent oscillatory solutions, one moving to the left and the other to the right. In the previous nondegenerate case only one solution is retained, since the other one diverges as $x \to +\infty$ and it has to be rejected.

In contrast to bound states, unbound states cannot be normalized and we cannot use boundary conditions.

4.2.3 Mixed Spectrum

Potentials that confine the particle for only some energies give rise to mixed spectra; the motion of the particle for such potentials is confined for some energy values only. For instance, for the potential displayed in Figure 4.1, if the energy of the particle is between $V_{min} < E < V_1$, the motion of the particle is confined (bound) and its spectrum is discrete, but if $E > V_2$, the particle's motion is unbound and its spectrum is continuous (if $V_1 < E < V_2$, the motion is unbound only along the $x = -\infty$ direction). Other typical examples where mixed spectra are encountered are the finite square well potential and the Coulomb or molecular potential.

4.2.4 Symmetric Potentials and Parity

Most of the potentials that are encountered at the microscopic level are symmetric (or even) with respect to space inversion, $\hat{V}(-x) = \hat{V}(x)$. This symmetry introduces considerable simplifications in the calculations.

When $\hat{V}(x)$ is even, the corresponding Hamiltonian, $\hat{H}(x) = -(\hbar^2/2m)d^2/dx^2 + \hat{V}(x)$, is also even. We saw in Chapter 2 that even operators commute with the parity operator; hence they can have a common eigenbasis.

Let us consider the following two cases pertaining to degenerate and nondegenerate spectra of this Hamiltonian:

- **Nondegenerate spectrum**

  First we consider the particular case where the eigenvalues of the Hamiltonian corresponding to this symmetric potential are not degenerate. According to Theorem 4.1, this Hamiltonian describes bound states. We saw in Chapter 2 that a nondegenerate, even operator has the same eigenstates as the parity operator. Since the eigenstates of the parity operator have definite parity, *the bound eigenstates of a particle moving in a one-dimensional symmetric potential have definite parity; they are either even or odd*:

$$\boxed{\hat{V}(-x) = \hat{V}(x) \quad \Longrightarrow \quad \psi(-x) = \pm\psi(x).} \tag{4.4}$$

- **Degenerate spectrum**

  If the spectrum of the Hamiltonian corresponding to a symmetric potential is degenerate, the eigenstates are expressed only in terms of even and odd states. That is, the eigenstates do not have definite parity.

Summary: The various properties of the one-dimensional motion discussed in this section can be summarized as follows:

- The energy spectrum of a bound state system is discrete and nondegenerate.
- The bound state wave function $\psi_n(x)$ has: (a) n nodes if $n = 0$ corresponds to the ground state and (b) $(n-1)$ nodes if $n = 1$ corresponds to the ground state.
- The bound state eigenfunctions in an even potential have definite parity.
- The eigenfunctions of a degenerate spectrum in an even potential do not have definite parity.

4.3 The Free Particle: Continuous States

This is the simplest one-dimensional problem; it corresponds to $V(x) = 0$ for any value of x. In this case the Schrödinger equation is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \qquad \Longrightarrow \qquad \left(\frac{d^2}{dx^2} + k^2\right)\psi(x) = 0, \tag{4.5}$$

where $k^2 = 2mE/\hbar^2$, k being the wave number. The most general solution to (4.5) is a combination of two linearly independent *plane waves* $\psi_+(x) = e^{ikx}$ and $\psi_-(x) = e^{-ikx}$:

$$\psi_k(x) = A_+e^{ikx} + A_-e^{-ikx}, \tag{4.6}$$

where A_+ and A_- are two arbitrary constants. The complete wave function is thus given by the stationary state

$$\Psi_k(x,t) = A_+ e^{i(kx-\omega t)} + A_- e^{-i(kx+\omega t)} = A_+ e^{i(kx-\hbar k^2 t/2m)} + A_- e^{-i(kx+\hbar k^2 t/2m)}, \quad (4.7)$$

since $\omega = E/\hbar = \hbar k^2/2m$. The first term, $\Psi_+(x,t) = A_+ e^{i(kx-\omega t)}$, represents a wave traveling to the right, while the second term, $\Psi_-(x,t) = A_- e^{-i(kx+\omega t)}$, represents a wave traveling to the left. The intensities of these waves are given by $|A_+|^2$ and $|A_-|^2$, respectively. We should note that the waves $\Psi_+(x,t)$ and $\Psi_-(x,t)$ are associated, respectively, with a free particle traveling to the right and to the left with *well-defined* momenta and energy: $p_\pm = \pm\hbar k$, $E_\pm = \hbar^2 k^2/2m$. We will comment on the physical implications of this in a moment. Since there are no boundary conditions, there are no restrictions on k or on E; all values yield solutions to the equation.

The free particle problem is simple to solve mathematically, yet it presents a number of physical subtleties. Let us discuss briefly three of these subtleties. First, the probability densities corresponding to either solutions

$$P_\pm(x,t) = |\Psi_\pm(x,t)|^2 = |A_\pm|^2 \quad (4.8)$$

are constant, for they depend neither on x nor on t. This is due to the complete loss of information about the position and time for a state with definite values of momentum, $p_\pm = \pm\hbar k$, and energy, $E_\pm = \hbar^2 k^2/2m$. This is a consequence of Heisenberg's uncertainty principle: when the momentum and energy of a particle are known exactly, $\Delta p = 0$ and $\Delta E = 0$, there must be total uncertainty about its position and time: $\Delta x \longrightarrow \infty$ and $\Delta t \longrightarrow \infty$. The second subtlety pertains to an apparent discrepancy between the speed of the wave and the speed of the particle it is supposed to represent. The speed of the plane waves $\Psi_\pm(x,t)$ is given by

$$v_{wave} = \frac{\omega}{k} = \frac{E}{\hbar k} = \frac{\hbar^2 k^2/2m}{\hbar k} = \frac{\hbar k}{2m}. \quad (4.9)$$

On the other hand, the classical speed of the particle[2] is given by

$$v_{classical} = \frac{p}{m} = \frac{\hbar k}{m} = 2v_{wave}. \quad (4.10)$$

This means that the particle travels twice as fast as the wave that represents it! Third, the wave function is not normalizable:

$$\int_{-\infty}^{+\infty} \Psi_\pm^*(x,t)\Psi_\pm(x,t)\,dx = |A_\pm|^2 \int_{-\infty}^{+\infty} dx \to \infty. \quad (4.11)$$

The solutions $\Psi_\pm(x,t)$ are thus unphysical; physical wave functions must be square integrable. The problem can be traced to this: a free particle cannot have sharply defined momenta and energy.

In view of the three subtleties outlined above, the solutions of the Schrödinger equation (4.5) that are physically acceptable cannot be plane waves. Instead, we can construct physical

[2]The classical speed can be associated with the flux (or current density) which, as shown in Chapter 3, is $J_+ = i\hbar\frac{1}{2m}(\Psi_+\frac{\partial\Psi_+^*}{\partial x} - \Psi_+^*\frac{\partial\Psi_+}{\partial x}) = \frac{\hbar k}{m} = \frac{p}{m}$, where use was made of $A_+ = 1$.

solutions by means of a linear superposition of plane waves. The answer is provided by *wave packets*, which we have seen in Chapter 1:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i(kx-\omega t)} dk, \tag{4.12}$$

where $\phi(k)$, the amplitude of the wave packet, is given by the Fourier transform of $\psi(x,0)$ as

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi(x,0) e^{-ikx} dx. \tag{4.13}$$

The wave packet solution cures and avoids all the subtleties raised above. First, the momentum, the position and the energy of the particle are no longer known exactly; only probabilistic outcomes are possible. Second, as shown in Chapter 1, the wave packet (4.12) and the particle travel with the same speed $v_g = p/m$, called the *group* speed or the speed of the whole packet. Third, the wave packet (4.12) is normalizable.

To summarize, a free particle cannot be represented by a single (monochromatic) plane wave; it has to be represented by a wave packet. The physical solutions of the Schrödinger equation are thus given by wave packets, not by stationary solutions.

4.4 The Potential Step

Another simple problem consists of a particle that is free everywhere, but beyond a particular point, say $x = 0$, the potential increases sharply (i.e., it becomes repulsive or attractive). A potential of this type is called a potential step (see Figure 4.2):

$$V(x) = \begin{cases} 0, & x < 0, \\ V_0, & x \geq 0. \end{cases} \tag{4.14}$$

In this problem we try to analyze the dynamics of a flux of particles (all having the same mass m and moving with the same velocity) moving from left to the right. We are going to consider two cases, depending on whether the energy of the particles is larger or smaller than V_0.

(a) Case $E > V_0$

The particles are free for $x < 0$ and feel a repulsive potential V_0 that starts at $x = 0$ and stays flat (constant) for $x > 0$. Let us analyze the dynamics of this flux of particles classically and then quantum mechanically.

Classically, the particles approach the potential step or barrier from the left with a constant momentum $\sqrt{2mE}$. As the particles enter the region $x \geq 0$, where the potential now is $V = V_0$, they slow down to a momentum $\sqrt{2m(E - V_0)}$; they will then conserve this momentum as they travel to the right. Since the particles have sufficient energy to penetrate into the region $x \geq 0$, there will be *total transmission*: all the particles will emerge to the right with a smaller kinetic energy $E - V_0$. This is then a simple *scattering* problem in one dimension.

Quantum mechanically, the dynamics of the particle is regulated by the Schrödinger equation, which is given in these two regions by

$$\left(\frac{d^2}{dx^2} + k_1^2\right) \psi_1(x) = 0 \qquad (x < 0), \tag{4.15}$$

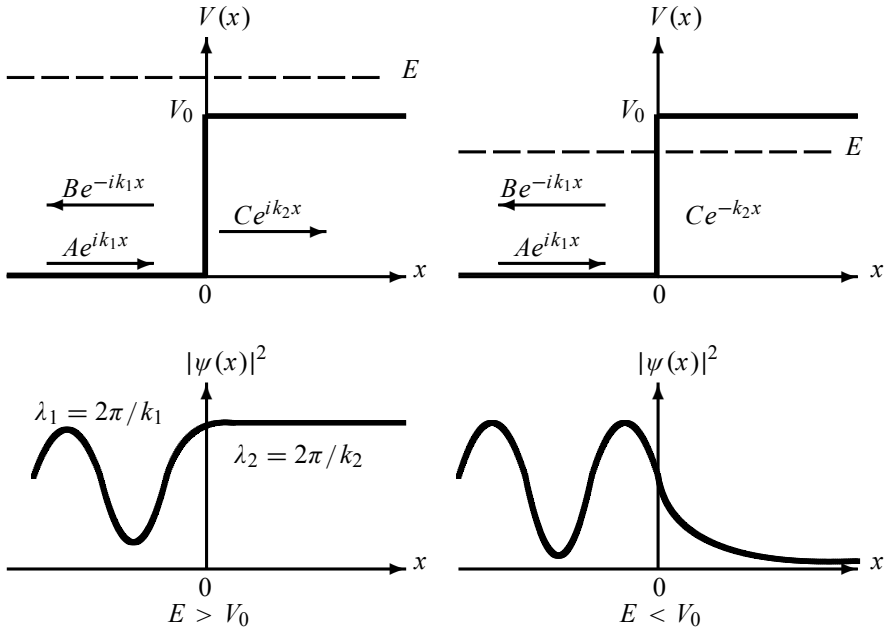


Figure 4.2 Potential step and propagation directions of the incident, reflected, and transmitted waves, plus their probability densities $|\psi(x)|^2$ when $E > V_0$ and $E < V_0$.

$$\left(\frac{d^2}{dx^2} + k_2^2\right)\psi_2(x) = 0 \qquad (x \geq 0), \tag{4.16}$$

where $k_1^2 = 2mE/\hbar^2$ and $k_2^2 = 2m(E - V_0)/\hbar^2$. The most general solutions to these two equations are plane waves:

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \qquad (x < 0), \tag{4.17}$$

$$\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x} \qquad (x \geq 0), \tag{4.18}$$

where Ae^{ik_1x} and Ce^{ik_2x} represent waves moving in the positive x-direction, but Be^{-ik_1x} and De^{-ik_2x} correspond to waves moving in the negative x-direction. We are interested in the case where the particles are initially incident on the potential step from the left: they can be reflected or transmitted at $x = 0$. Since no wave is reflected from the region $x > 0$ to the left, the constant D must vanish. Since we are dealing with stationary states, the complete wave function is thus given by

$$\Psi(x,t) = \begin{cases} \psi_1(x)e^{-i\omega t} = Ae^{i(k_1x-\omega t)} + Be^{-i(k_1x+\omega t)} & x < 0 \\ \psi_2(x)e^{-i\omega t} = Ce^{i(k_2x-\omega t)} & x \geq 0, \end{cases} \tag{4.19}$$

where $A\exp[i(k_1x-\omega t)]$, $B\exp[-i(k_1x+\omega t)]$, and $C\exp[i(k_2x-\omega t)]$ represent the *incident*, the *reflected*, and the *transmitted* waves, respectively; they travel to the right, the left, and the right (Figure 4.2). Note that the probability density $|\psi(x)|^2$ shown in the lower left plot of Figure 4.2 is a straight line for $x > 0$, since $|\psi_2(x)|^2 = |C\exp i(k_2x - \omega t)|^2 = |C|^2$.

Let us now evaluate the *reflection* and *transmission coefficients*, R and T, as defined by

$$R = \left|\frac{\text{reflected current density}}{\text{incident current density}}\right| = \left|\frac{J_{reflected}}{J_{incident}}\right|, \qquad T = \left|\frac{J_{transmitted}}{J_{incident}}\right|; \tag{4.20}$$

R represents the ratio of the reflected to the incident beams and T the ratio of the transmitted to the incident beams. To calculate R and T, we need to find $J_{incident}$, $J_{reflected}$, and $J_{transmitted}$. Since the incident wave is $\psi_i(x) = Ae^{ik_1x}$, the incident current density (or incident flux) is given by

$$J_{incident} = \frac{i\hbar}{2m}\left(\psi_i(x)\frac{d\psi_i^*(x)}{dx} - \psi_i^*(x)\frac{d\psi_i(x)}{dx}\right) = \frac{\hbar k_1}{m}|A|^2. \tag{4.21}$$

Similarly, since the reflected and transmitted waves are $\psi_r(x) = Be^{-ik_1x}$ and $\psi_t(x) = Ce^{ik_2x}$, we can verify that the reflected and transmitted fluxes are

$$J_{reflected} = -\frac{\hbar k_1}{m}|B|^2, \qquad J_{transmitted} = \frac{\hbar k_2}{m}|C|^2. \tag{4.22}$$

A combination of (4.20) to (4.22) yields

$$R = \frac{|B|^2}{|A|^2}, \qquad T = \frac{k_2}{k_1}\frac{|C|^2}{|A|^2}. \tag{4.23}$$

Thus, the calculation of R and T is reduced to determining the constants B and C. For this, we need to use the boundary conditions of the wave function at $x = 0$. Since both the wave function and its first derivative are continuous at $x = 0$,

$$\psi_1(0) = \psi_2(0), \qquad \frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx}, \tag{4.24}$$

equations (4.17) and (4.18) yield

$$A + B = C, \qquad k_1(A - B) = k_2C; \tag{4.25}$$

hence

$$B = \frac{k_1 - k_2}{k_1 + k_2}A, \qquad C = \frac{2k_1}{k_1 + k_2}A. \tag{4.26}$$

As for the constant A, it can be determined from the normalization condition of the wave function, but we don't need it here, since R and T are expressed in terms of ratios. A combination of (4.23) with (4.26) leads to

$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} = \frac{(1 - \mathcal{K})^2}{(1 + \mathcal{K})^2}, \qquad T = \frac{4k_1k_2}{(k_1 + k_2)^2} = \frac{4\mathcal{K}}{(1 + \mathcal{K})^2}, \tag{4.27}$$

where $\mathcal{K} = k_2/k_1 = \sqrt{1 - V_0/E}$. The sum of R and T is equal to 1, as it should be.

In contrast to classical mechanics, which states that none of the particles get reflected, equation (4.27) shows that the quantum mechanical reflection coefficient R is not zero: there are particles that get reflected in spite of their energies being higher than the step V_0. This effect must be attributed to the *wavelike behavior* of the particles.

From (4.27) we see that as E gets smaller and smaller, T also gets smaller and smaller so that when $E = V_0$ the transmission coefficient T becomes zero and $R = 1$. On the other hand, when $E \gg V_0$, we have $\mathcal{K} = \sqrt{1 - V_0/E} \simeq 1$; hence $R = 0$ and $T = 1$. This is expected since, when the incident particles have very high energies, the potential step is so weak that it produces no noticeable effect on their motion.

Remark: physical meaning of the boundary conditions

Throughout this chapter, we will encounter at numerous times the use of the boundary conditions of the wave function and its first derivative as in Eq (4.24). What is the underlying physics behind these continuity conditions? We can make two observations:

- Since the probability density $|\psi(x)|^2$ of finding the particle in any small region varies continuously from one point to another, the wave function $\psi(x)$ must, therefore, be a continuous function of x; thus, as shown in (4.24), we must have $\psi_1(0) = \psi_2(0)$.
- Since the linear momentum of the particle, $\hat{P}\psi(x) = -i\hbar d\psi(x)/dx$, must be a continuous function of x as the particle moves from left to right, the first derivative of the wave function, $d\psi(x)/dx$, must also be a continuous function of x, notably at $x = 0$. Hence, as shown in (4.24), we must have $d\psi_1(0)/dx = d\psi_2(0)/dx$.

(b) Case $E < V_0$

Classically, the particles arriving at the potential step from the left (with momenta $p = \sqrt{2mE}$) will come to a stop at $x = 0$ and then all will bounce back to the left with the magnitudes of their momenta unchanged. None of the particles will make it into the right side of the barrier $x = 0$; there is total reflection of the particles. So the motion of the particles is reversed by the potential barrier.

Quantum mechanically, the picture will be somewhat different. In this case, the Schrödinger equation and the wave function in the region $x < 0$ are given by (4.15) and (4.17), respectively. But for $x > 0$ the Schrödinger equation is given by

$$\left(\frac{d^2}{dx^2} - k_2'^2\right)\psi_2(x) = 0 \quad (x \geq 0), \tag{4.28}$$

where $k_2'^2 = 2m(V_0 - E)/\hbar^2$. This equation's solution is

$$\psi_2(x) = Ce^{-k_2'x} + De^{k_2'x} \quad (x \geq 0). \tag{4.29}$$

Since the wave function must be finite everywhere, and since the term $e^{k_2'x}$ diverges when $x \to \infty$, the constant D has to be zero. Thus, the complete wave function is

$$\Psi(x,t) = \begin{cases} Ae^{i(k_1x-\omega t)} + Be^{-i(k_1x+\omega t)}, & x < 0, \\ Ce^{-k_2'x}e^{-i\omega t}, & x \geq 0. \end{cases} \tag{4.30}$$

Let us now evaluate, as we did in the previous case, the reflected and the transmitted coefficients. First we should note that the transmitted coefficient, which corresponds to the transmitted wave function $\psi_t(x) = Ce^{-k_2'x}$, is zero since $\psi_t(x)$ is a *purely real* function ($\psi_t^*(x) = \psi_t(x)$) and therefore

$$J_{transmitted} = \frac{\hbar}{2im}\left(\psi_t(x)\frac{d\psi_t(x)}{dx} - \psi_t(x)\frac{d\psi_t(x)}{dx}\right) = 0. \tag{4.31}$$

Hence, the reflected coefficient R must be equal to 1. We can obtain this result by applying the continuity conditions at $x = 0$ for (4.17) and (4.29):

$$B = \frac{k_1 - ik_2'}{k_1 + ik_2'}A, \qquad C = \frac{2k_1}{k_1 + ik_2'}A. \tag{4.32}$$

Thus, the reflected coefficient is given by

$$R = \frac{|B|^2}{|A|^2} = \frac{k_1^2 + k_2'^2}{k_1^2 + k_2'^2} = 1. \tag{4.33}$$

We therefore have total reflection, as in the classical case.

There is, however, a difference with the classical case: while none of the particles can be found classically in the region $x > 0$, quantum mechanically there is a *nonzero probability* that the wave function penetrates this *classically forbidden* region. To see this, note that the relative probability density

$$P(x) = |\psi_t(x)|^2 = |C|^2 e^{-2k_2' x} = \frac{4k_1^2 |A|^2}{k_1^2 + k_2'^2} e^{-2k_2' x} \tag{4.34}$$

is appreciable near $x = 0$ and falls exponentially to small values as x becomes large; the behavior of the probability density is shown in Figure 4.2.

4.5 The Potential Barrier and Well

Consider a beam of particles of mass m that are sent from the left on a potential barrier

$$V(x) = \begin{cases} 0, & x < 0, \\ V_0, & 0 \le x \le a, \\ 0, & x > a. \end{cases} \tag{4.35}$$

This potential, which is repulsive, supports no bound states (Figure 4.3). We are dealing here, as in the case of the potential step, with a one-dimensional *scattering* problem.

Again, let us consider the following two cases which correspond to the particle energies being respectively larger and smaller than the potential barrier.

4.5.1 The Case $E > V_0$

Classically, the particles that approach the barrier from the left at constant momentum, $p_1 = \sqrt{2mE}$, as they enter the region $0 \le x \le a$ will slow down to a momentum $p_2 = \sqrt{2m(E - V_0)}$. They will maintain the momentum p_2 until they reach the point $x = a$. Then, as soon as they pass beyond the point $x = a$, they will accelerate to a momentum $p_3 = \sqrt{2mE}$ and maintain this value in the entire region $x > a$. Since the particles have enough energy to cross the barrier, none of the particles will be reflected back; all the particles will emerge on the right side of $x = a$: *total transmission*.

It is easy to infer the quantum mechanical study from the treatment of the potential step presented in the previous section. We need only to mention that the wave function will display an oscillatory pattern in all three regions; its amplitude reduces every time the particle enters a new region (see Figure 4.3):

$$\psi(x) = \begin{cases} \psi_1(x) = Ae^{ik_1 x} + Be^{-ik_1 x}, & x \le 0, \\ \psi_2(x) = Ce^{ik_2 x} + De^{-ik_2 x}, & 0 < x < a, \\ \psi_3(x) = Ee^{ik_1 x}, & x \ge a, \end{cases} \tag{4.36}$$

where $k_1 = \sqrt{2mE/\hbar^2}$ and $k_2 = \sqrt{2m(E - V_0)/\hbar^2}$. The constants B, C, D, and E can be obtained in terms of A from the boundary conditions: $\psi(x)$ and $d\psi/dx$ must be continuous at $x = 0$ and $x = a$, respectively:

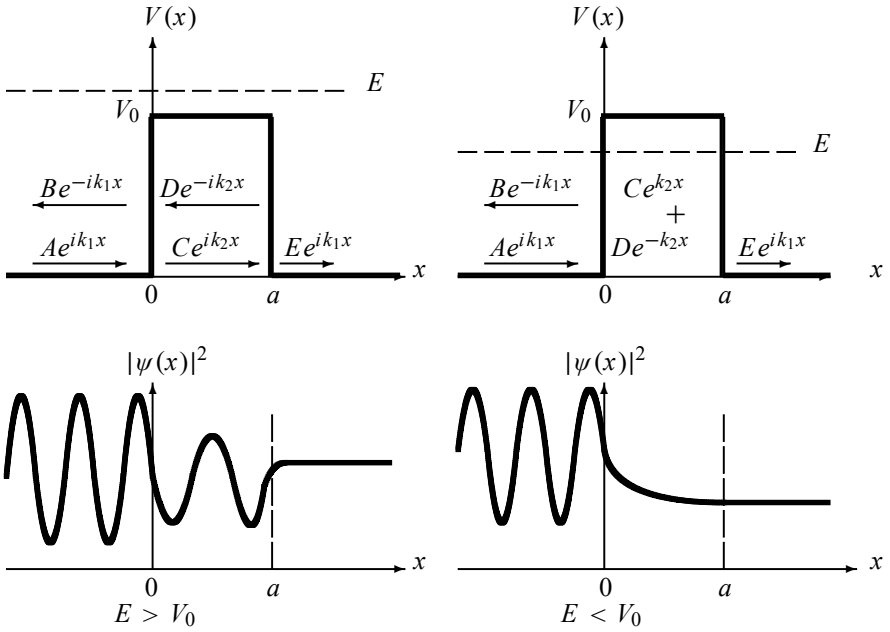


Figure 4.3 Potential barrier and propagation directions of the incident, reflected, and transmitted waves, plus their probability densities $|\psi(x)|^2$ when $E > V_0$ and $E < V_0$.

$$\psi_1(0) = \psi_2(0), \qquad \frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx}, \tag{4.37}$$

$$\psi_2(a) = \psi_3(a), \qquad \frac{d\psi_2(a)}{dx} = \frac{d\psi_3(a)}{dx}. \tag{4.38}$$

These equations yield

$$A + B = C + D, \qquad ik_1(A - B) = ik_2(C - D), \tag{4.39}$$

$$Ce^{ik_2a} + De^{-ik_2a} = Ee^{ik_1a}, \qquad ik_2\left(Ce^{ik_2a} - De^{-ik_2a}\right) = ik_1Ee^{ik_1a}. \tag{4.40}$$

Solving for E, we obtain

$$\begin{aligned} E &= 4k_1k_2Ae^{-ik_1a}[(k_1 + k_2)^2 e^{-ik_2a} - (k_1 - k_2)^2 e^{ik_2a}]^{-1} \\ &= 4k_1k_2Ae^{-ik_1a}\left[4k_1k_2\cos(k_2a) - 2i\left(k_1^2 + k_2^2\right)\sin(k_2a)\right]^{-1}. \end{aligned} \tag{4.41}$$

The transmission coefficient is thus given by

$$\begin{aligned} T &= \frac{k_1|E|^2}{k_1|A|^2} = \left[1 + \frac{1}{4}\left(\frac{k_1^2 - k_2^2}{k_1k_2}\right)^2 \sin^2(k_2a)\right]^{-1} \\ &= \left[1 + \frac{V_0^2}{4E(E - V_0)}\sin^2\left(a\sqrt{2mV_0/\hbar^2}\sqrt{E/V_0 - 1}\right)\right]^{-1}, \end{aligned} \tag{4.42}$$

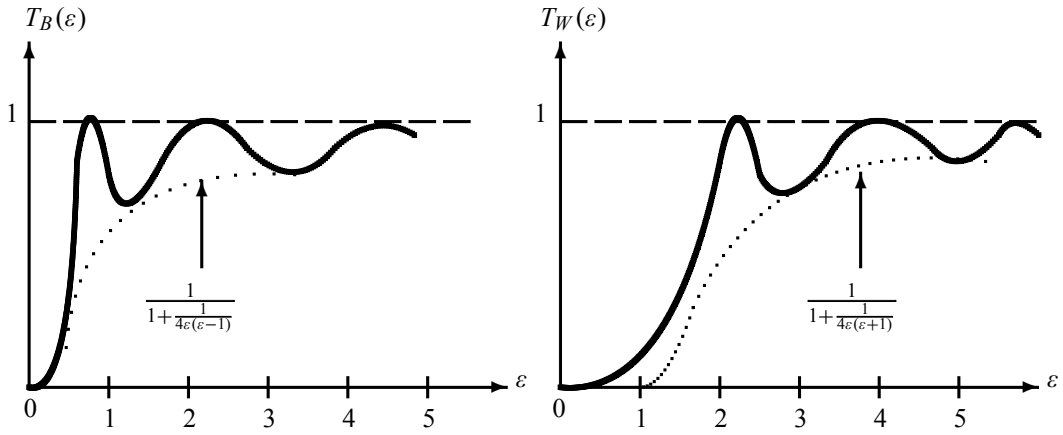


Figure 4.4 Transmission coefficients for a potential barrier, $T_B(\varepsilon) = \frac{4\varepsilon(\varepsilon-1)}{4\varepsilon(\varepsilon-1)+\sin^2(\lambda\sqrt{\varepsilon-1})}$, and for a potential well, $T_W(\varepsilon) = \frac{4\varepsilon(\varepsilon+1)}{4\varepsilon(\varepsilon+1)+\sin^2(\lambda\sqrt{\varepsilon+1})}$.

because

$$\left(\frac{k_1^2 - k_2^2}{k_1 k_2}\right)^2 = \frac{V_0^2}{E(E - V_0)}. \tag{4.43}$$

Using the notation $\lambda = a\sqrt{2mV_0/\hbar^2}$ and $\varepsilon = E/V_0$, we can rewrite T as

$$T = \left[1 + \frac{1}{4\varepsilon(\varepsilon - 1)} \sin^2(\lambda\sqrt{\varepsilon - 1})\right]^{-1}. \tag{4.44}$$

Similarly, we can show that

$$R = \frac{\sin^2(\lambda\sqrt{\varepsilon - 1})}{4\varepsilon(\varepsilon - 1) + \sin^2(\lambda\sqrt{\varepsilon - 1})} = \left[1 + \frac{4\varepsilon(\varepsilon - 1)}{\sin^2(\lambda\sqrt{\varepsilon - 1})}\right]^{-1}. \tag{4.45}$$

Special cases

- If $E \gg V_0$, and hence $\varepsilon \gg 1$, the transmission coefficient T becomes asymptotically equal to unity, $T \simeq 1$, and $R \simeq 0$. So, at very high energies and weak potential barrier, the particles would not feel the effect of the barrier; we have total transmission.
- We also have total transmission when $\sin(\lambda\sqrt{\varepsilon - 1}) = 0$ or $\lambda\sqrt{\varepsilon - 1} = n\pi$. As shown in Figure 4.4, the total transmission, $T(\varepsilon_n) = 1$, occurs whenever $\varepsilon_n = E_n/V_0 = n^2\pi^2\hbar^2/(2ma^2V_0) + 1$ or whenever the incident energy of the particle is $E_n = V_0 + n^2\pi^2\hbar^2/(2ma^2)$ with $n = 1, 2, 3, \ldots$. The maxima of the transmission coefficient coincide with the energy eigenvalues of the infinite square well potential; these are known as resonances. This resonance phenomenon, which does not occur in classical physics, results from a constructive interference between the incident and the reflected waves. This phenomenon is observed experimentally in a number of cases such as when scattering low-energy ($E \sim 0.1$ eV) electrons off noble atoms (known as the *Ramsauer–Townsend effect*, a consequence of symmetry of noble atoms) and neutrons off nuclei.

- In the limit $\varepsilon \to 1$ we have $\sin(\lambda\sqrt{\varepsilon-1}) \sim \lambda\sqrt{\varepsilon-1}$, hence (4.44) and (4.45) become

$$T = \left(1 + \frac{ma^2V_0}{2\hbar^2}\right)^{-1}, \qquad R = \left(1 + \frac{2\hbar^2}{ma^2V_0}\right)^{-1}. \tag{4.46}$$

The potential well ($V_0 < 0$)
The transmission coefficient (4.44) was derived for the case where $V_0 > 0$, i.e., for a *barrier potential*. Following the same procedure that led to (4.44), we can show that the transmission coefficient for a finite *potential well*, $V_0 < 0$, is given by

$$T_W = \left[1 + \frac{1}{4\varepsilon(\varepsilon+1)}\sin^2(\lambda\sqrt{\varepsilon+1})\right]^{-1}, \tag{4.47}$$

where $\varepsilon = E/|V_0|$ and $\lambda = a\sqrt{2m|V_0|/\hbar^2}$. Notice that there is total transmission whenever $\sin(\lambda\sqrt{\varepsilon+1}) = 0$ or $\lambda\sqrt{\varepsilon+1} = n\pi$. As shown in Figure 4.4, the total transmission, $T_W(\varepsilon_n) = 1$, occurs whenever $\varepsilon_n = E_n/|V_0| = n^2\pi^2\hbar^2/(2ma^2V_0) - 1$ or whenever the incident energy of the particle is $E_n = n^2\pi^2\hbar^2/(2ma^2) - |V_0|$ with $n = 1, 2, 3, \ldots$. We will study in more detail the *symmetric* potential well in Section 4.7.

4.5.2 The Case $E < V_0$: Tunneling

Classically, we would expect total reflection: every particle that arrives at the barrier ($x = 0$) will be reflected back; no particle can penetrate the barrier, where it would have a negative kinetic energy.

We are now going to show that the quantum mechanical predictions differ sharply from their classical counterparts, for the wave function is not zero beyond the barrier. The solutions of the Schrödinger equation in the three regions yield expressions that are similar to (4.36) except that $\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}$ should be replaced with $\psi_2(x) = Ce^{k_2x} + De^{-k_2x}$:

$$\psi(x) = \begin{cases} \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}, & x \le 0, \\ \psi_2(x) = Ce^{k_2x} + De^{-k_2x}, & 0 < x < a, \\ \psi_3(x) = Ee^{ik_1x}, & x \ge a, \end{cases} \tag{4.48}$$

where $k_1^2 = 2mE/\hbar^2$ and $k_2^2 = 2m(V_0 - E)/\hbar^2$. The behavior of the probability density corresponding to this wave function is expected, as displayed in Figure 4.3, to be oscillatory in the regions $x < 0$ and $x > a$, and exponentially decaying for $0 \le x \le a$.

To find the reflection and transmission coefficients,

$$R = \frac{|B|^2}{|A|^2}, \qquad T = \frac{|E|^2}{|A|^2}, \tag{4.49}$$

we need only to calculate B and E in terms of A. The continuity conditions of the wave function and its derivative at $x = 0$ and $x = a$ yield

$$A + B = C + D, \tag{4.50}$$

$$ik_1(A - B) = k_2(C - D), \tag{4.51}$$

$$Ce^{k_2a} + De^{-k_2a} = Ee^{ik_1a}, \tag{4.52}$$

$$k_2\left(Ce^{k_2a} - De^{-k_2a}\right) = ik_1Ee^{ik_1a}. \tag{4.53}$$

The last two equations lead to the following expressions for C and D:

$$C = \frac{E}{2}\left(1 + i\frac{k_1}{k_2}\right)e^{(ik_1-k_2)a}, \qquad D = \frac{E}{2}\left(1 - i\frac{k_1}{k_2}\right)e^{(ik_1+k_2)a}. \tag{4.54}$$

Inserting these two expressions into the two equations (4.50) and (4.51) and dividing by A, we can show that these two equations reduce, respectively, to

$$1 + \frac{B}{A} = \frac{E}{A}e^{ik_1a}\left[\cosh(k_2a) - i\frac{k_1}{k_2}\sinh(k_2a)\right], \tag{4.55}$$

$$1 - \frac{B}{A} = \frac{E}{A}e^{ik_1a}\left[\cosh(k_2a) + i\frac{k_2}{k_1}\sinh(k_2a)\right]. \tag{4.56}$$

Solving these two equations for B/A and E/A, we obtain

$$\frac{B}{A} = -i\frac{k_1^2+k_2^2}{k_1k_2}\sinh(k_2a)\left[2\cosh(k_2a) + i\frac{k_2^2-k_1^2}{k_1k_2}\sinh(k_2a)\right]^{-1}, \tag{4.57}$$

$$\frac{E}{A} = 2e^{-ik_1a}\left[2\cosh(k_2a) + i\frac{k_2^2-k_1^2}{k_1k_2}\sinh(k_2a)\right]^{-1}. \tag{4.58}$$

Thus, the coefficients R and T become

$$R = \left(\frac{k_1^2+k_2^2}{k_1k_2}\right)^2\sinh^2(k_2a)\left[4\cosh^2(k_2a) + \left(\frac{k_2^2-k_1^2}{k_1k_2}\right)^2\sinh^2(k_2a)\right]^{-1}, \tag{4.59}$$

$$T = \frac{|E|^2}{|A|^2} = 4\left[4\cosh^2(k_2a) + \left(\frac{k_2^2-k_1^2}{k_1k_2}\right)^2\sinh^2(k_2a)\right]^{-1}. \tag{4.60}$$

We can rewrite R in terms of T as

$$R = \frac{1}{4}T\left(\frac{k_1^2+k_2^2}{k_1k_2}\right)^2\sinh^2(k_2a). \tag{4.61}$$

Since $\cosh^2(k_2a) = 1 + \sinh^2(k_2a)$ we can reduce (4.60) to

$$T = \left[1 + \frac{1}{4}\left(\frac{k_1^2+k_2^2}{k_1k_2}\right)^2\sinh^2(k_2a)\right]^{-1}. \tag{4.62}$$

Note that T is *finite*. This means that the probability for the transmission of the particles into the region $x \geq a$ is *not zero* (in classical physics, however, the particle can in no way make it into the $x \geq 0$ region). This is a purely quantum mechanical effect which is due to the *wave aspect* of microscopic objects; it is known as the *tunneling effect*: *quantum mechanical objects can tunnel through classically impenetrable barriers*. This *barrier penetration* effect has important applications in various branches of modern physics ranging from particle and nuclear physics

to semiconductor devices. For instance, radioactive decays and charge transport in electronic devices are typical examples of the tunneling effect.

Now since

$$\left(\frac{k_1^2+k_2^2}{k_1k_2}\right)^2=\left(\frac{V_0}{\sqrt{E(V_0-E)}}\right)^2=\frac{V_0^2}{E(V_0-E)}, \tag{4.63}$$

we can rewrite (4.61) and (4.62) as follows:

$$R=\frac{1}{4}\frac{V_0^2T}{E(V_0-E)}\sinh^2\left(\frac{a}{\hbar}\sqrt{2m(V_0-E)}\right), \tag{4.64}$$

$$T=\left[1+\frac{1}{4}\frac{V_0^2}{E(V_0-E)}\sinh^2\left(\frac{a}{\hbar}\sqrt{2m(V_0-E)}\right)\right]^{-1}, \tag{4.65}$$

or

$$R=\frac{T}{4\varepsilon(1-\varepsilon)}\sinh^2\left(\lambda\sqrt{1-\varepsilon}\right), \tag{4.66}$$

$$T=\left[1+\frac{1}{4\varepsilon(1-\varepsilon)}\sinh^2\left(\lambda\sqrt{1-\varepsilon}\right)\right]^{-1}, \tag{4.67}$$

where $\lambda=a\sqrt{2mV_0/\hbar^2}$ and $\varepsilon=E/V_0$.

Special cases

- If $E\ll V_0$, hence $\varepsilon\ll 1$ or $\lambda\sqrt{1-\varepsilon}\gg 1$, we may approximate $\sinh\left(\lambda\sqrt{1-\varepsilon}\right)\simeq\frac{1}{2}\exp\left(\lambda\sqrt{1-\varepsilon}\right)$. We can thus show that the transmission coefficient (4.67) becomes asymptotically equal to

$$\begin{aligned}T &\simeq \left\{\frac{1}{4\varepsilon(1-\varepsilon)}\left[\frac{1}{2}e^{\lambda\sqrt{1-\varepsilon}}\right]^2\right\}^{-1}=16\varepsilon(1-\varepsilon)e^{-2\lambda\sqrt{1-\varepsilon}}\\ &= \frac{16E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-(2a/\hbar)\sqrt{2m(V_0-E)}}.\end{aligned} \tag{4.68}$$

  This shows that the transmission coefficient is not zero, as it would be classically, but has a finite value. So, quantum mechanically, there is a finite tunneling beyond the barrier, $x>a$.

- When $E\simeq V_0$, hence $\varepsilon\simeq 1$, we can verify that (4.66) and (4.67) lead to the relations (4.46).

- Taking the classical limit $\hbar\to 0$, the coefficients (4.66) and (4.67) reduce to the classical result: $R\to 1$ and $T\to 0$.

4.5.3 The Tunneling Effect

In general, the tunneling effect consists of the propagation of a particle through a region where the particle's energy is smaller than the potential energy $E<V(x)$. Classically this region, defined by $x_1<x<x_2$ (Figure 4.5a), is forbidden to the particle where its kinetic energy

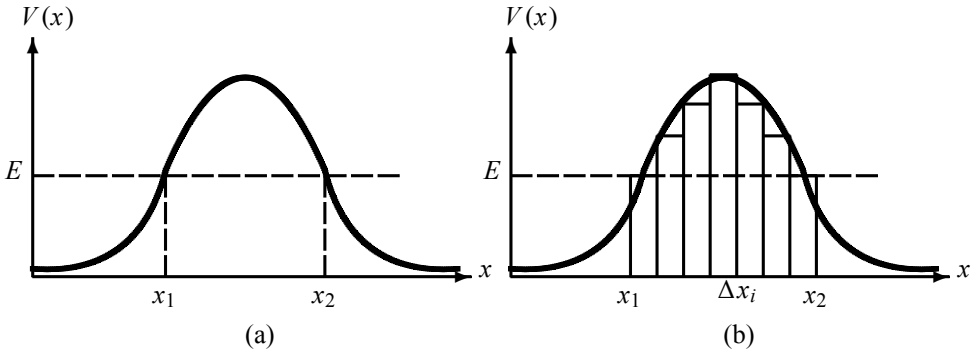


Figure 4.5 (a) Tunneling though a potential barrier. (b) Approximation of a smoothly varying potential $V(x)$ by square barriers.

would be negative; the points $x = x_1$ and $x = x_2$ are known as the *classical turning points*. Quantum mechanically, however, since particles display wave features, the quantum waves can tunnel through the barrier.

As shown in the square barrier example, the particle has a finite probability of tunneling through the barrier. In this case we managed to find an analytical expression (4.67) for the tunneling probability only because we dealt with a simple square potential. Analytic expressions cannot be obtained for potentials with arbitrary spatial dependence. In such cases one needs approximations. The Wentzel–Kramers–Brillouin (WKB) method (Chapter 9) provides one of the most useful approximation methods. We will show that the transmission coefficient for a barrier potential $V(x)$ is given by

$$T \sim \exp\left\{-\frac{2}{\hbar}\int_{x_1}^{x_2} dx\sqrt{2m\,[V(x)-E]}\right\}. \tag{4.69}$$

We can obtain this relation by means of a crude approximation. For this, we need simply to take the classically forbidden region $x_1 < x < x_2$ (Figure 4.5b) and divide it into a series of small intervals Δx_i. If Δx_i is small enough, we may approximate the potential $V(x_i)$ at each point x_i by a square potential barrier. Thus, we can use (4.68) to calculate the transmission probability corresponding to $V(x_i)$:

$$T_i \sim \exp\left[-\frac{2\Delta x_i}{\hbar}\sqrt{2m(V(x_i)-E)}\right]. \tag{4.70}$$

The transmission probability for the general potential of Figure 4.5, where we divided the region $x_1 < x < x_2$ into a very large number of small intervals Δx_i, is given by

$$\begin{aligned} T \quad &\sim \quad \lim_{N\to\infty}\prod_{i=1}^{N}\exp\left[-\frac{2\Delta x_i}{\hbar}\sqrt{2m(V(x_i)-E)}\right] \\ &= \quad \exp\left[-\frac{2}{\hbar}\lim_{\Delta x_i\to 0}\sum_i \Delta x_i\sqrt{2m(V(x_i)-E)}\right] \\ &\longrightarrow \quad \exp\left[-\frac{2}{\hbar}\int_{x_1}^{x_2} dx\sqrt{2m\,[V(x)-E]}\right]. \end{aligned} \tag{4.71}$$

The approximation leading to this relation is valid, as will be shown in Chapter 9, only if the potential $V(x)$ is a smooth, slowly varying function of x.

4.6 The Infinite Square Well Potential

4.6.1 The Asymmetric Square Well

Consider a particle of mass m confined to move inside an infinitely deep asymmetric potential well

$$V(x) = \begin{cases} +\infty, & x < 0, \\ 0, & 0 \le x \le a, \\ +\infty, & x > a. \end{cases} \tag{4.72}$$

Classically, the particle remains confined inside the well, moving at constant momentum $p = \pm\sqrt{2mE}$ back and forth as a result of repeated reflections from the walls of the well.

Quantum mechanically, we expect this particle to have only bound state solutions and a discrete nondegenerate energy spectrum. Since $V(x)$ is infinite outside the region $0 \le x \le a$, the wave function of the particle must be zero outside the boundary. Hence we can look for solutions only inside the well

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0, \tag{4.73}$$

with $k^2 = 2mE/\hbar^2$; the solutions are

$$\psi(x) = A'e^{ikx} + B'e^{-ikx} \quad \Longrightarrow \quad \psi(x) = A\sin(kx) + B\cos(kx). \tag{4.74}$$

The wave function vanishes at the walls, $\psi(0) = \psi(a) = 0$: the condition $\psi(0) = 0$ gives $B = 0$, while $\psi(a) = A\sin(ka) = 0$ gives

$$k_n a = n\pi \qquad (n = 1, 2, 3, \cdots). \tag{4.75}$$

This condition determines the energy

$$\boxed{E_n = \frac{\hbar^2}{2m}k_n^2 = \frac{\hbar^2\pi^2}{2ma^2}n^2 \qquad (n = 1, 2, 3, \cdots).} \tag{4.76}$$

The energy is *quantized*; only certain values are permitted. This is expected since the states of a particle which is confined to a limited region of space are *bound states* and the energy spectrum is *discrete*. This is in sharp contrast to classical physics where the energy of the particle, given by $E = p^2/(2m)$, takes any value; the classical energy evolves *continuously*.

As it can be inferred from (4.76), we should note that the energy between adjacent levels is not constant:

$$E_{n+1} - E_n = 2n + 1, \tag{4.77}$$

which leads to

$$\frac{E_{n+1} - E_n}{E_n} = \frac{(n+1)^2 - n^2}{n^2} = \frac{2n+1}{n^2}. \tag{4.78}$$

In the classical limit $n \to \infty$,

$$\lim_{n\to\infty} \frac{E_{n+1} - E_n}{E_n} = \lim_{n\to\infty} \frac{2n+1}{n^2} = 0, \tag{4.79}$$

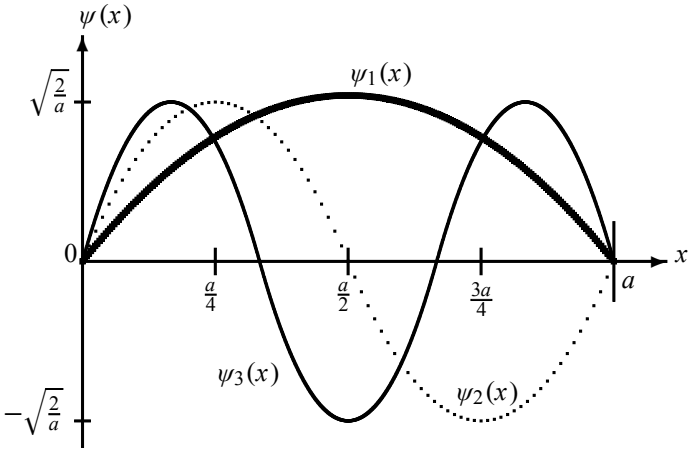


Figure 4.6 Three lowest states of an infinite potential well, $\psi_n(x) = \sqrt{2/a}\sin(n\pi x/a)$; the states $\psi_{2n+1}(x)$ and $\psi_{2n}(x)$ are even and odd, respectively, with respect to $x = a/2$.

the levels become so close together as to be practically indistinguishable.

Since $B = 0$ and $k_n = n\pi/a$, (4.74) yields $\psi_n(x) = A\sin(n\pi x/a)$. We can choose the constant A so that $\psi_n(x)$ is normalized:

$$1 = \int_0^a |\psi_n(x)|^2 dx = |A|^2 \int_0^a \sin^2\left(\frac{n\pi}{a}x\right) dx \quad \Longrightarrow \quad A = \sqrt{\frac{2}{a}}, \tag{4.80}$$

hence

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) \qquad (n = 1, 2, 3, \cdots).} \tag{4.81}$$

The first few functions are plotted in Figure 4.6.

The solution of the time-independent Schrödinger equation has thus given us the energy (4.76) and the wave function (4.81). There is then an infinite sequence of discrete energy levels corresponding to the positive integer values of the *quantum number* n. It is clear that $n = 0$ yields an uninteresting result: $\psi_0(x) = 0$ and $E_0 = 0$; later, we will examine in more detail the physical implications of this. So, the lowest energy, or *ground state* energy, corresponds to $n = 1$; it is $E_1 = \hbar^2\pi^2/(2ma^2)$. As will be explained later, this is called the *zero-point energy*, for there exists no state with zero energy. The states corresponding to $n = 2, 3, 4, \ldots$ are called *excited states*; their energies are given by $E_n = n^2 E_1$. As mentioned in Theorem 4.2, each function $\psi_n(x)$ has $(n-1)$ nodes. Figure 4.6 shows that the functions $\psi_{2n+1}(x)$ are even and the functions $\psi_{2n}(x)$ are odd with respect to the center of the well; we will study this in Section 4.6.2 when we consider the symmetric potential well. Note that none of the energy levels is degenerate (there is only one eigenfunction for each energy level) and that the wave functions corresponding to different energy levels are orthogonal:

$$\int_0^a \psi_m^*(x)\psi_n(x)\,dx = \delta_{mn}. \tag{4.82}$$

Since we are dealing with stationary states and since $E_n = n^2 E_1$, the most general solutions of

the time-dependent Schrödinger equation are given by

$$\Psi(x,t)=\sum_{n=1}^{\infty}\psi_n(x)e^{-iE_nt/\hbar}=\sqrt{\frac{2}{a}}\sum_{n=1}^{\infty}\sin\left(\frac{n\pi x}{a}\right)e^{-in^2E_1t/\hbar}. \tag{4.83}$$

Zero-point energy

Let us examine why there is no state with zero energy for a square well potential. If the particle has zero energy, it will be at rest inside the well, and this violates Heisenberg's uncertainty principle. By *localizing* or confining the particle to a limited region in space, it will acquire a *finite* momentum leading to a minimum kinetic energy. That is, the localization of the particle's motion to $0 \le x \le a$ implies a position uncertainty of order $\Delta x \sim a$ which, according to the uncertainty principle, leads to a minimum momentum uncertainty $\Delta p \sim \hbar/a$ and this in turn leads to a minimum kinetic energy of order $\hbar^2/(2ma^2)$. This is in qualitative agreement with the exact value $E_1 = \pi^2\hbar^2/(2ma^2)$. In fact, as will be shown in (4.216), an accurate evaluation of Δp_1 leads to a zero-point energy which is equal to E_1.

Note that, as the momentum uncertainty is inversely proportional to the width of the well, $\Delta p \sim \hbar/a$, if the width decreases (i.e., the particle's position is confined further and further), the uncertainty on $\hat{P}$ will increase. This makes the particle move faster and faster, so the zero-point energy will also increase. Conversely, if the width of the well increases, the zero-point energy decreases, but it will never vanish.

The zero-point energy therefore reflects the necessity of a *minimum motion* of a particle due to localization. The zero-point energy occurs in all bound state potentials. In the case of binding potentials, the lowest energy state has an energy which is higher than the minimum of the potential energy. This is in sharp contrast to classical mechanics, where the lowest possible energy is equal to the minimum value of the potential energy, with zero kinetic energy. In quantum mechanics, however, the lowest state does not minimize the potential alone, but applies to the sum of the kinetic and potential energies, and this leads to a finite ground state or zero-point energy. This concept has far-reaching physical consequences in the realm of the microscopic world. For instance, without the zero-point motion, atoms would not be stable, for the electrons would fall into the nuclei. Also, it is the zero-point energy which prevents helium from freezing at very low temperatures.

The following example shows that the zero-point energy is also present in macroscopic systems, but it is infinitesimally small. In the case of microscopic systems, however, it has a nonnegligible size.

Example 4.1 (Zero-point energy)

To illustrate the idea that the zero-point energy gets larger by going from macroscopic to microscopic systems, calculate the zero-point energy for a particle in an infinite potential well for the following three cases:

(a) a 100 g ball confined on a 5 m long line,

(b) an oxygen atom confined to a 2×10^{-10} m lattice, and

(c) an electron confined to a 10^{-10} m atom.

Solution

(a) The zero-point energy of a 100 g ball that is confined to a 5 m long line is

$$E=\frac{\hbar^2\pi^2}{2ma^2}\simeq\frac{10\times10^{-68}\,\text{J}}{2\times0.1\times25}\simeq2\times10^{-68}\,\text{J}=1.25\times10^{-49}\,\text{eV}. \tag{4.84}$$

This energy is too small to be detected, much less measured, by any known experimental technique.

(b) For the zero-point energy of an oxygen atom confined to a 2×10^{-10} m lattice, since the oxygen atom has 16 nucleons, its mass is of the order of $m \simeq 16 \times 1.6 \times 10^{-27}$ kg $\simeq 26 \times 10^{-27}$ kg, so we have

$$E = \frac{10^{-67}\,\text{J}}{2 \times 26 \times 10^{-27} \times 4 \times 10^{-20}} \simeq 0.5 \times 10^{-22}\,\text{J} \simeq 3 \times 10^{-4}\,\text{eV}. \tag{4.85}$$

(c) The zero-point energy of an electron ($m \sim 10^{-30}$ kg) that is confined to an atom ($a \sim 1 \times 10^{-10}$ m) is

$$E = \frac{10^{-67}\,\text{J}}{2 \times 10^{-30} \times 10^{-20}} \simeq 5 \times 10^{-18}\,\text{J} \simeq 30\,\text{eV}. \tag{4.86}$$

This energy is important at the atomic scale, for the binding energy of a hydrogen electron is about 14 eV. So the zero-point energy is negligible for macroscopic objects, but important for microscopic systems.

4.6.2 The Symmetric Potential Well

What happens if the potential (4.72) is translated to the left by a distance of $a/2$ to become symmetric?

$$V(x) = \begin{cases} +\infty, & x < -a/2, \\ 0, & -a/2 \le x \le a/2, \\ +\infty, & x > a/2. \end{cases} \tag{4.87}$$

First, we would expect the energy spectrum (4.76) to remain unaffected by this translation, since the Hamiltonian is invariant under spatial translations; as it contains only a kinetic part, it commutes with the particle's momentum, $[\hat{H}, \hat{P}] = 0$. The energy spectrum is discrete and nondegenerate.

Second, earlier in this chapter we saw that for symmetric potentials, $V(-x) = V(x)$, the wave function of bound states must be either even or odd. The wave function corresponding to the potential (4.87) can be written as follows:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left[\frac{n\pi}{a}\left(x + \frac{a}{2}\right)\right] = \begin{cases} \sqrt{\frac{2}{a}} \cos(\frac{n\pi}{a}x) & (n = 1, 3, 5, 7, \cdots), \\ \sqrt{\frac{2}{a}} \sin(\frac{n\pi}{a}x) & (n = 2, 4, 6, 8, \cdots). \end{cases} \tag{4.88}$$

That is, the wave functions corresponding to odd quantum numbers $n = 1, 3, 5, \ldots$ are symmetric, $\psi(-x) = \psi(x)$, and those corresponding to even numbers $n = 2, 4, 6, \ldots$ are antisymmetric, $\psi(-x) = -\psi(x)$.

4.7 The Finite Square Well Potential

Consider a particle of mass m moving in the following symmetric potential:

$$V(x) = \begin{cases} V_0, & x < -a/2, \\ 0, & -a/2 \le x \le a/2, \\ V_0, & x > a/2. \end{cases} \tag{4.89}$$

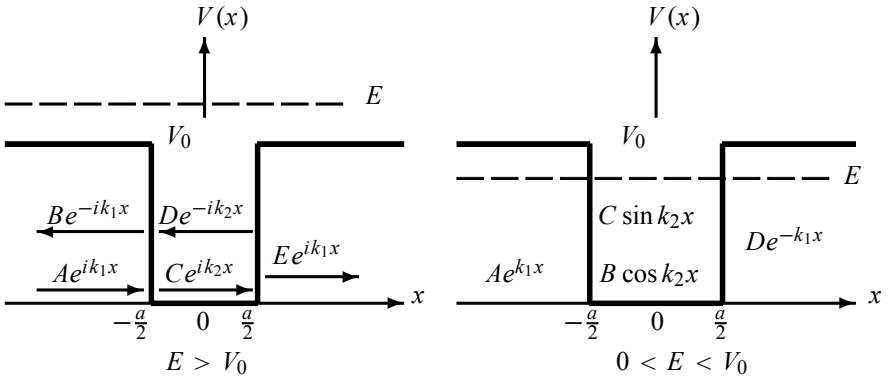


Figure 4.7 Finite square well potential and propagation directions of the incident, reflected and transmitted waves when $E > V_0$ and $0 < E < V_0$.

The two physically interesting cases are $E > V_0$ and $E < V_0$ (see Figure 4.7). We expect the solutions to yield a *continuous* doubly-degenerate energy spectrum for $E > V_0$ and a *discrete* nondegenerate spectrum for $0 < E < V_0$.

4.7.1 The Scattering Solutions ($E > V_0$)

Classically, if the particle is initially incident from left with constant momentum $\sqrt{2m(E - V_0)}$, it will speed up to $\sqrt{2mE}$ between $-a/2 \leq x \leq a/2$ and then slow down to its initial momentum in the region $x > a$. All the particles that come from the left will be transmitted, none will be reflected back; therefore $T = 1$ and $R = 0$.

Quantum mechanically, and as we did for the step and barrier potentials, we can verify that we get a *finite* reflection coefficient. The solution is straightforward to obtain; just follow the procedure outlined in the previous two sections. The wave function has an oscillating pattern in all three regions (see Figure 4.7).

4.7.2 The Bound State Solutions ($0 < E < V_0$)

Classically, when $E < V_0$ the particle is completely confined to the region $-a/2 \leq x \leq a/2$; it will bounce back and forth between $x = -a/2$ and $x = a/2$ with constant momentum $p = \sqrt{2mE}$.

Quantum mechanically, the solutions are particularly interesting for they are expected to yield a *discrete* energy spectrum and wave functions that decay in the two regions $x < -a/2$ and $x > a/2$, but oscillate in $-a/2 \leq x \leq a/2$. In these three regions, the Schrödinger equation can be written as

$$\left(\frac{d^2}{dx^2} - k_1^2\right)\psi_1(x) = 0 \qquad \left(x < -\frac{1}{2}a\right), \tag{4.90}$$

$$\left(\frac{d^2}{dx^2} + k_2^2\right)\psi_2(x) = 0 \qquad \left(-\frac{1}{2}a \leq x \leq \frac{1}{2}a\right), \tag{4.91}$$

$$\left(\frac{d^2}{dx^2} - k_1^2\right)\psi_3(x) = 0 \qquad \left(x > \frac{1}{2}a\right), \tag{4.92}$$

where $k_1^2 = 2m(V_0 - E)/\hbar^2$ and $k_2^2 = 2mE/\hbar^2$. Eliminating the physically unacceptable solutions which grow exponentially for large values of $|x|$, we can write the solution to this Schrödinger equation in the regions $x < -a/2$ and $x > a/2$ as follows:

$$\psi_1(x) = Ae^{k_1 x} \qquad \left(x < -\frac{1}{2}a\right), \tag{4.93}$$

$$\psi_3(x) = De^{-k_1 x} \qquad \left(x > \frac{1}{2}a\right). \tag{4.94}$$

As mentioned in (4.4), since the bound state eigenfunctions of symmetric one-dimensional Hamiltonians are either even or odd under space inversion, the solutions of (4.90) to (4.92) are then either antisymmetric (odd)

$$\psi_a(x) = \begin{cases} Ae^{k_1 x}, & x < -a/2, \\ C\sin(k_2 x), & -a/2 \le x \le a/2, \\ De^{-k_1 x}, & x > a/2, \end{cases} \tag{4.95}$$

or symmetric (even)

$$\psi_s(x) = \begin{cases} Ae^{k_1 x}, & x < -a/2, \\ B\cos(k_2 x), & -a/2 \le x \le a/2, \\ De^{-k_1 x}, & x > a/2. \end{cases} \tag{4.96}$$

To determine the eigenvalues, we need to use the continuity conditions at $x = \pm a/2$. The continuity of the logarithmic derivative, $(1/\psi_a(x))d\psi_a(x)/dx$, of $\psi_a(x)$ at $x = \pm a/2$ yields

$$k_2 \cot\left(\frac{k_2 a}{2}\right) = -k_1. \tag{4.97}$$

Similarly, the continuity of $(1/\psi_s(x))d\psi_s(x)/dx$ at $x = \pm a/2$ gives

$$k_2 \tan\left(\frac{k_2 a}{2}\right) = k_1. \tag{4.98}$$

The transcendental equations (4.97) and (4.98) cannot be solved directly; we can solve them either graphically or numerically. To solve these equations graphically, we need only to rewrite them in the following suggestive forms:

$$-\alpha_n \cot\alpha_n = \sqrt{R^2 - \alpha_n^2} \qquad \text{(for odd states)}, \tag{4.99}$$

$$\alpha_n \tan\alpha_n = \sqrt{R^2 - \alpha_n^2} \qquad \text{(for even states)}, \tag{4.100}$$

where $\alpha_n^2 = (k_2 a/2)^2 = ma^2 E_n/(2\hbar^2)$ and $R^2 = ma^2 V_0/(2\hbar^2)$; these equations are obtained by inserting $k_1 = \sqrt{2m(V_0 - E)/\hbar^2}$ and $k_2 = \sqrt{2mE/\hbar^2}$ into (4.97) and (4.98). The left-hand sides of (4.99) and (4.100) consist of trigonometric functions; the right-hand sides consist of a circle of radius R. The solutions are given by the points where the circle $\sqrt{R^2 - \alpha_n^2}$ intersects the functions $-\alpha_n \cot\alpha_n$ and $\alpha_n \tan\alpha_n$ (Figure 4.8). The solutions form a *discrete* set. As illustrated in Figure 4.8, the intersection of the small circle with the curve $\alpha_n \tan\alpha_n$ yields only one bound state, $n = 0$, whereas the intersection of the larger circle with $\alpha_n \tan\alpha_n$ yields two

bound states, $n = 0, 2$, and its intersection with $-\alpha_n \cot \alpha_n$ yields two other bound states, $n = 1,\ 3$.

The number of solutions depends on the size of R, which in turn depends on the depth V_0 and the width a of the well, since $R = \sqrt{ma^2 V_0/(2\hbar^2)}$. The deeper and broader the well, the larger the value of R, and hence the greater the number of bound states. Note that there is always at least one bound state (i.e., one intersection) no matter how small V_0 is. When

$$0 < R < \frac{\pi}{2} \qquad \text{or} \qquad 0 < V_0 < \left(\frac{\pi}{2}\right)^2 \frac{2\hbar^2}{ma^2}, \tag{4.101}$$

there is only one bound state corresponding to $n = 0$ (see Figure 4.8); this state—the ground state—is even. Then, and when

$$\frac{\pi}{2} < R < \pi \qquad \text{or} \qquad \left(\frac{\pi}{2}\right)^2 \frac{2\hbar^2}{ma^2} < V_0 < \pi^2 \frac{2\hbar^2}{ma^2}, \tag{4.102}$$

there are two bound states: an even state (the ground state) corresponding to $n = 0$ and the first odd state corresponding to $n = 1$. Now, if

$$\pi < R < \frac{3\pi}{2} \qquad \text{or} \qquad \pi^2 \frac{2\hbar^2}{ma^2} < V_0 < \left(\frac{3\pi}{2}\right)^2 \frac{2\hbar^2}{ma^2}, \tag{4.103}$$

there exist three bound states: the ground state (even state), $n = 0$, the first excited state (odd state), corresponding to $n = 1$, and the second excited state (even state), which corresponds to $n = 2$. In general, the well width at which n states are allowed is given by

$$R = \frac{n\pi}{2} \qquad \text{or} \qquad V_0 = \left(\frac{\pi}{2}\right)^2 \frac{2\hbar^2}{ma^2} n^2. \tag{4.104}$$

The spectrum, therefore, consists of a set of alternating even and odd states: the lowest state, the ground state, is even, the next state (first excited sate) is odd, and so on.

In the limiting case $V_0 \to \infty$, the circle's radius R also becomes infinite, and hence the function $\sqrt{R^2 - \alpha_n^2}$ will cross $-\alpha_n \cot \alpha_n$ and $\alpha_n \tan \alpha_n$ at the asymptotes $\alpha_n = n\pi/2$, because when $V_0 \to \infty$ both $\tan \alpha_n$ and $\cot \alpha_n$ become infinite:

$$\tan \alpha_n \to \infty \quad \Longrightarrow \quad \alpha_n = \frac{2n+1}{2}\pi \qquad (n = 0, 1, 2, 3, \cdots), \tag{4.105}$$

$$\cot \alpha_n \to \infty \quad \Longrightarrow \quad \alpha_n = n\pi \qquad (n = 1, 2, 3, \cdots). \tag{4.106}$$

Combining these two cases, we obtain

$$\alpha_n = \frac{n\pi}{2} \qquad (1, 2, 3, \ldots). \tag{4.107}$$

Since $\alpha_n^2 = ma^2 E_n/(2\hbar^2)$ we see that we recover the energy expression for the infinite well:

$$\alpha_n = \frac{n\pi}{2} \longrightarrow E_n = \frac{\pi^2 \hbar^2}{2ma^2} n^2. \tag{4.108}$$

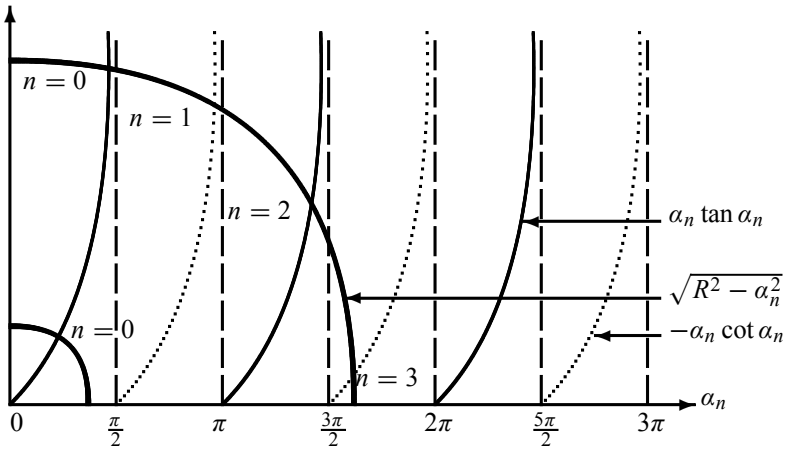


Figure 4.8 Graphical solutions for the finite square well potential: they are given by the intersections of $\sqrt{R^2-\alpha_n^2}$ with $\alpha_n \tan\alpha_n$ and $-\alpha_n \cot\alpha_n$, where $\alpha_n^2 = ma^2E_n/(2\hbar^2)$ and $R^2 = ma^2V_0/(2\hbar^2)$.

Example 4.2
Find the number of bound states and the corresponding energies for the finite square well potential when: (a) $R = 1$ (i.e., $\sqrt{ma^2V_0/(2\hbar^2)} = 1$), and (b) $R = 2$.

Solution

(a) From Figure 4.8, when $R = \sqrt{ma^2V_0/(2\hbar^2)} = 1$, there is only one bound state since $\alpha_n \leq R$. This bound state corresponds to $n = 0$. The corresponding energy is given by the intersection of $\alpha_0 \tan\alpha_0$ with $\sqrt{1-\alpha_0^2}$:

$$\alpha_0 \tan\alpha_0 = \sqrt{1-\alpha_0^2} \quad \Longrightarrow \quad \alpha_0^2(1+\tan^2\alpha_0) = 1 \quad \Longrightarrow \quad \cos^2\alpha_0 = \alpha_0^2. \tag{4.109}$$

The solution of $\cos^2\alpha_0 = \alpha_0^2$ is given numerically by $\alpha_0 = 0.739\,09$. Thus, the corresponding energy is determined by the relation $\sqrt{ma^2E_0/(2\hbar^2)} = 0.739\,09$, which yields $E_0 \simeq 1.1\hbar^2/(ma^2)$.

(b) When $R = 2$ there are two bound states resulting from the intersections of $\sqrt{4-\alpha_0^2}$ with $\alpha_0 \tan\alpha_0$ and $-\alpha_1 \cot\alpha_1$; they correspond to $n = 0$ and $n = 1$, respectively. The numerical solutions of the corresponding equations

$$\alpha_0 \tan\alpha_0 = \sqrt{4-\alpha_0^2} \quad \Longrightarrow \quad 4\cos^2\alpha_0 = \alpha_0^2, \tag{4.110}$$

$$-\alpha_1 \cot\alpha_1 = \sqrt{4-\alpha_1^2} \quad \Longrightarrow \quad 4\sin^2\alpha_1 = \alpha_1^2, \tag{4.111}$$

yield $\alpha_0 \simeq 1.03$ and $\alpha_1 \simeq 1.9$, respectively. The corresponding energies are

$$\alpha_0 = \sqrt{\frac{ma^2E_0}{2\hbar^2}} \simeq 1.03 \quad \Longrightarrow \quad E_0 \simeq \frac{2.12\hbar^2}{ma^2}, \tag{4.112}$$

$$\alpha_1 = \sqrt{\frac{ma^2E_1}{2\hbar^2}} \simeq 1.9 \quad \Longrightarrow \quad E_1 \simeq \frac{7.22\hbar^2}{ma^2}. \tag{4.113}$$

4.8 The Harmonic Oscillator

The harmonic oscillator is one of those few problems that are important to all branches of physics. It provides a useful model for a variety of vibrational phenomena that are encountered, for instance, in classical mechanics, electrodynamics, statistical mechanics, solid state, atomic, nuclear, and particle physics. In quantum mechanics, it serves as an invaluable tool to illustrate the basic concepts and the formalism.

The Hamiltonian of a particle of mass m which oscillates with an angular frequency ω under the influence of a one-dimensional harmonic potential is

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{1}{2}m\omega^2\hat{X}^2. \tag{4.114}$$

The problem is how to find the energy eigenvalues and eigenstates of this Hamiltonian. This problem can be studied by means of two separate methods. The first method, called the *analytic method*, consists in solving the time-independent Schrödinger equation (TISE) for the Hamiltonian (4.114). The second method, called the *ladder* or *algebraic method*, does not deal with solving the Schrödinger equation, but deals instead with operator algebra involving operators known as the *creation* and *annihilation* or *ladder* operators; this method is in essence a matrix formulation, because it expresses the various quantities in terms of matrices. In our presentation, we are going to adopt the second method, for it is more straightforward, more elegant and much simpler than solving the Schrödinger equation. Unlike the examples seen up to now, solving the Schrödinger equation for the potential $V(x) = \frac{1}{2}m\omega x^2$ is no easy job. Before embarking on the second method, let us highlight the main steps involved in the first method.

Brief outline of the analytic method

This approach consists in using the power series method to solve the following differential (Schrödinger) equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}m\omega^2x^2\psi(x) = E\psi(x), \tag{4.115}$$

which can be reduced to

$$\frac{d^2\psi(x)}{dx^2} + \left(\frac{2mE}{\hbar^2} - \frac{x^2}{x_0^4}\right)\psi(x) = 0, \tag{4.116}$$

where $x_0 = \sqrt{\hbar/(m\omega)}$ is a constant that has the dimensions of length; it sets the length scale of the oscillator, as will be seen later. The solutions of differential equations like (4.116) have been worked out by our mathematician colleagues well before the arrival of quantum mechanics (the solutions are expressed in terms of some special functions, the Hermite polynomials). The occurrence of the term $x^2\psi(x)$ in (4.116) suggests trying a Gaussian type solution[3]: $\psi(x) =$

[3] Solutions of the type $\psi(x) = f(x)\exp(x^2/2x_0^2)$ are physically unacceptable, for they diverge when $x \longrightarrow \pm\infty$.

$f(x)\exp(-x^2/2x_0^2)$, where $f(x)$ is a function of x. Inserting this trial function into (4.116), we obtain a differential equation for $f(x)$. This new differential equation can be solved by expanding $f(x)$ out in a power series (i.e., $f(x) = \sum_{n=0}^{\infty} a_n x^n$, where a_n is just a coefficient), which when inserted into the differential equation leads to a recursion relation. By demanding the power series of $f(x)$ to terminate at some finite value of n (because the wave function $\psi(x)$ has to be finite everywhere, notably when $x \longrightarrow \pm\infty$), the recursion relation yields an expression for the energy eigenvalues which are discrete or quantized:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad (n = 0, 1, 2, 3, \ \ldots). \tag{4.117}$$

After some calculations, we can show that the wave functions that are physically acceptable and that satisfy (4.116) are given by

$$\psi_n(x) = \frac{1}{\sqrt{\sqrt{\pi}2^n n! x_0}} e^{-x^2/2x_0^2} H_n\left(\frac{x}{x_0}\right), \tag{4.118}$$

where $H_n(y)$ are nth order polynomials called *Hermite polynomials*:

$$H_n(y) = (-1)^n e^{y^2} \frac{d^n}{dy^n} e^{-y^2}. \tag{4.119}$$

From this relation it is easy to calculate the first few polynomials:

$$\begin{aligned} &H_0(y) = 1, && H_1(y) = 2y, \\ &H_2(y) = 4y^2 - 2, && H_3(y) = 8y^3 - 12y, \\ &H_4(y) = 16y^4 - 48y^2 + 12, && H_5(y) = 32y^5 - 160y^3 + 120y. \end{aligned} \tag{4.120}$$

We will deal with the physical interpretations of the harmonic oscillator results when we study the second method.

Algebraic method

Let us now show how to solve the harmonic oscillator eigenvalue problem using the algebraic method. For this, we need to rewrite the Hamiltonian (4.114) in terms of the two Hermitian, dimensionless operators $\hat{p} = \hat{P}/\sqrt{m\hbar\omega}$ and $\hat{q} = \hat{X}\sqrt{m\omega/\hbar}$:

$$\hat{H} = \frac{\hbar\omega}{2}(\hat{p}^2 + \hat{q}^2), \tag{4.121}$$

and then introduce two non-Hermitian, dimensionless operators:

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{q} + i\,\hat{p}), \qquad \hat{a}^\dagger = \frac{1}{\sqrt{2}}(\hat{q} - i\,\hat{p}). \tag{4.122}$$

The physical meaning of the operators $\hat{a}$ and $\hat{a}^\dagger$ will be examined later. Note that

$$\hat{a}^\dagger\hat{a} = \frac{1}{2}(\hat{q} - i\,\hat{p})(\hat{q} + i\,\hat{p}) = \frac{1}{2}(\hat{q}^2 + \hat{p}^2 + i\hat{q}\,\hat{p} - i\,\hat{p}\hat{q}) = \frac{1}{2}(\hat{q}^2 + \hat{p}^2) + \frac{i}{2}[\hat{q},\ \hat{p}], \tag{4.123}$$

where, using $[\hat{X}, \hat{P}] = i\hbar$, we can verify that the commutator between $\hat{q}$ and $\hat{p}$ is

$$[\hat{q},\ \hat{p}] = \left[\sqrt{\frac{m\omega}{\hbar}}\hat{X}, \frac{1}{\sqrt{\hbar m\omega}}\hat{P}\right] = \frac{1}{\hbar}\left[\hat{X}, \hat{P}\right] = i; \tag{4.124}$$

hence

$$\hat{a}^\dagger \hat{a} = \frac{1}{2}(\hat{q}^2 + \hat{p}^2) - \frac{1}{2} \tag{4.125}$$

or

$$\frac{1}{2}(\hat{q}^2 + \hat{p}^2) = \hat{a}^\dagger \hat{a} + \frac{1}{2}. \tag{4.126}$$

Inserting (4.126) into (4.121) we obtain

$$\boxed{\hat{H} = \hbar\omega\left(\hat{a}^\dagger \hat{a} + \frac{1}{2}\right) = \hbar\omega\left(\hat{N} + \frac{1}{2}\right) \qquad \text{with} \quad \hat{N} = \hat{a}^\dagger \hat{a},} \tag{4.127}$$

where $\hat{N}$ is known as the *number* operator or *occupation number* operator, which is clearly Hermitian.

Let us now derive the commutator $[\hat{a}, \hat{a}^\dagger]$. Since $[\hat{X}, \hat{P}] = i\hbar$ we have $[\hat{q}, \hat{p}] = \frac{1}{\hbar}[\hat{X}, \hat{P}] = i$; hence

$$[\hat{a}, \hat{a}^\dagger] = \frac{1}{2}\left[\hat{q} + i\hat{p}, \hat{q} - i\hat{p}\right] = -i\left[\hat{q}, \hat{p}\right] = 1 \tag{4.128}$$

or

$$\boxed{[\hat{a}, \hat{a}^\dagger] = 1.} \tag{4.129}$$

4.8.1 Energy Eigenvalues

Note that $\hat{H}$ as given by (4.127) commutes with $\hat{N}$, since $\hat{H}$ is linear in $\hat{N}$. Thus, $\hat{H}$ and $\hat{N}$ can have a set of joint eigenstates, to be denoted by $\mid n\rangle$:

$$\hat{N} \mid n\rangle = n \mid n\rangle \tag{4.130}$$

and

$$\hat{H} \mid n\rangle = E_n \mid n\rangle; \tag{4.131}$$

the states $\mid n\rangle$ are called energy eigenstates. Combining (4.127) and (4.131), we obtain the energy eigenvalues at once:

$$\boxed{E_n = \left(n + \frac{1}{2}\right)\hbar\omega.} \tag{4.132}$$

We will show later that n is a *positive integer*; it cannot have negative values.

The physical meaning of the operators $\hat{a}$, $\hat{a}^\dagger$, and $\hat{N}$ can now be clarified. First, we need the following two commutators that can be extracted from (4.129) and (4.127):

$$\boxed{[\hat{a}, \hat{H}] = \hbar\omega\hat{a}, \qquad [\hat{a}^\dagger, \hat{H}] = -\hbar\omega\hat{a}^\dagger.} \tag{4.133}$$

These commutation relations along with (4.131) lead to

$$\hat{H}\left(\hat{a} \mid n\rangle\right) \quad = (\hat{a}\hat{H} - \hbar\omega\hat{a}) \mid n\rangle \quad = (E_n - \hbar\omega)\left(\hat{a} \mid n\rangle\right), \tag{4.134}$$

$$\hat{H}\left(\hat{a}^\dagger \mid n\rangle\right) \quad = (\hat{a}^\dagger\hat{H} + \hbar\omega\hat{a}^\dagger) \mid n\rangle \; = (E_n + \hbar\omega)\left(\hat{a}^\dagger \mid n\rangle\right). \tag{4.135}$$

Thus, $\hat{a} \mid n\rangle$ and $\hat{a}^\dagger \mid n\rangle$ are eigenstates of $\hat{H}$ with eigenvalues $(E_n - \hbar\omega)$ and $(E_n + \hbar\omega)$, respectively. So the actions of $\hat{a}$ and $\hat{a}^\dagger$ on $\mid n\rangle$ generate new energy states that are lower and

higher by one unit of $\hbar\omega$, respectively. As a result, $\hat{a}$ and $\hat{a}^\dagger$ are respectively known as the *lowering* and *raising* operators, or the *annihilation* and *creation* operators; they are also known as the *ladder* operators.

Let us now find out how the operators $\hat{a}$ and $\hat{a}^\dagger$ act on the energy eigenstates $\mid n\rangle$. Since $\hat{a}$ and $\hat{a}^\dagger$ do not commute with $\hat{N}$, the states $\mid n\rangle$ are eigenstates neither to $\hat{a}$ nor to $\hat{a}^\dagger$. Using (4.129) along with $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$, we can show that

$$\boxed{[\hat{N}, \hat{a}] = -\hat{a}, \qquad [\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger;} \tag{4.136}$$

hence $\hat{N}\hat{a} = \hat{a}(\hat{N} - 1)$ and $\hat{N}\hat{a}^\dagger = \hat{a}^\dagger(\hat{N} + 1)$. Combining these relations with (4.130), we obtain

$$\hat{N}\left(\hat{a} \mid n\rangle\right) = \hat{a}(\hat{N} - 1) \mid n\rangle = (n - 1)\left(\hat{a} \mid n\rangle\right), \tag{4.137}$$

$$\hat{N}\left(\hat{a}^\dagger \mid n\rangle\right) = \hat{a}^\dagger(\hat{N} + 1) \mid n\rangle = (n + 1)(\hat{a}^\dagger \mid n\rangle). \tag{4.138}$$

These relations reveal that $\hat{a} \mid n\rangle$ and $\hat{a}^\dagger \mid n\rangle$ are eigenstates of $\hat{N}$ with eigenvalues $(n - 1)$ and $(n + 1)$, respectively. This implies that when $\hat{a}$ and $\hat{a}^\dagger$ operate on $\mid n\rangle$, respectively, they decrease and increase n by one unit. That is, while the action of $\hat{a}$ on $\mid n\rangle$ generates a new state $\mid n - 1\rangle$ (i.e., $\hat{a} \mid n\rangle \sim \mid n - 1\rangle$), the action of $\hat{a}^\dagger$ on $\mid n\rangle$ generates $\mid n + 1\rangle$. Hence from (4.137) we can write

$$\hat{a} \mid n\rangle = c_n \mid n - 1\rangle, \tag{4.139}$$

where c_n is a constant to be determined from the requirement that the states $\mid n\rangle$ be normalized for all values of n. On the one hand, (4.139) yields

$$\left(\langle n \mid \hat{a}^\dagger\right) \cdot \left(\hat{a} \mid n\rangle\right) = \langle n \mid \hat{a}^\dagger\hat{a} \mid n\rangle = |c_n|^2 \langle n - 1 \mid n - 1\rangle = |c_n|^2 \tag{4.140}$$

and, on the other hand, (4.130) gives

$$\left(\langle n \mid \hat{a}^\dagger\right) \cdot \left(\hat{a} \mid n\rangle\right) = \langle n \mid \hat{a}^\dagger\hat{a} \mid n\rangle = n\langle n \mid n\rangle = n. \tag{4.141}$$

When combined, the last two equations yield

$$|c_n|^2 = n. \tag{4.142}$$

This implies that n, which is equal to the norm of $\hat{a} \mid n\rangle$ (see (4.141)), *cannot be negative*, $n \geq 0$, since the norm is a positive quantity. Substituting (4.142) into (4.139) we end up with

$$\boxed{\hat{a} \mid n\rangle = \sqrt{n} \mid n - 1\rangle.} \tag{4.143}$$

This equation shows that repeated applications of the operator $\hat{a}$ on $\mid n\rangle$ generate a sequence of eigenvectors $\mid n - 1\rangle$, $\mid n - 2\rangle$, $\mid n - 3\rangle$, ... Since $n \geq 0$ and since $\hat{a} \mid 0\rangle = 0$, this sequence has to terminate at $n = 0$; this is true if we start with an integer value of n. But if we start with a noninteger n, the sequence will not terminate; hence it leads to eigenvectors with negative values of n. But as shown above, since n cannot be negative, we conclude that n has to be a *nonnegative integer*.

Now, we can easily show, as we did for (4.143), that

$$\boxed{\hat{a}^\dagger \mid n\rangle = \sqrt{n+1} \mid n+1\rangle.} \tag{4.144}$$

This implies that repeated applications of $\hat{a}^\dagger$ on $\mid n\rangle$ generate an infinite sequence of eigenvectors $\mid n+1\rangle$, $\mid n+2\rangle$, $\mid n+3\rangle$, ... Since n is a positive integer, the energy spectrum of a harmonic oscillator as specified by (4.132) is therefore *discrete*:

$$\boxed{E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad (n = 0, 1, 2, 3, \ldots).} \tag{4.145}$$

This expression is similar to the one obtained from the first method (see Eq. (4.117)). The energy spectrum of the harmonic oscillator consists of energy levels that are equally spaced: $E_{n+1} - E_n = \hbar\omega$. This is Planck's famous equidistant energy idea—the energy of the radiation emitted by the oscillating charges (from the inside walls of the cavity) must come only in bundles (quanta) that are integral multiples of $\hbar\omega$—which, as mentioned in Chapter 1, led to the birth of quantum mechanics.

As expected for bound states of one-dimensional potentials, the energy spectrum is both discrete and nondegenerate. Once again, as in the case of the infinite square well potential, we encounter the zero-point energy phenomenon: the lowest energy eigenvalue of the oscillator is not zero but is instead equal to $E_0 = \hbar\omega/2$. It is called the *zero-point energy* of the oscillator, for it corresponds to $n = 0$. The zero-point energy of bound state systems cannot be zero, otherwise it would violate the uncertainty principle. For the harmonic oscillator, for instance, the classical minimum energy corresponds to $x = 0$ and $p = 0$; there would be no oscillations in this case. This would imply that we know simultaneously and with absolute precision both the position and the momentum of the system. This would contradict the uncertainty principle.

4.8.2 Energy Eigenstates

The algebraic or operator method can also be used to determine the energy eigenvectors. First, using (4.144), we see that the various eigenvectors can be written in terms of the ground state $\mid 0\rangle$ as follows:

$$\mid 1\rangle = \hat{a}^\dagger \mid 0\rangle, \tag{4.146}$$

$$\mid 2\rangle = \frac{1}{\sqrt{2}}\hat{a}^\dagger \mid 1\rangle = \frac{1}{\sqrt{2!}}\left(\hat{a}^\dagger\right)^2 \mid 0\rangle, \tag{4.147}$$

$$\mid 3\rangle = \frac{1}{\sqrt{3}}\hat{a}^\dagger \mid 2\rangle = \frac{1}{\sqrt{3!}}\left(\hat{a}^\dagger\right)^3 \mid 0\rangle, \tag{4.148}$$

$$\vdots$$

$$\mid n\rangle = \frac{1}{\sqrt{n}}\hat{a}^\dagger \mid n-1\rangle = \frac{1}{\sqrt{n!}}\left(\hat{a}^\dagger\right)^n \mid 0\rangle. \tag{4.149}$$

So, to find any excited eigenstate $\mid n\rangle$, we need simply to operate $\hat{a}^\dagger$ on $\mid 0\rangle$ n successive times.

Note that any set of kets $\mid n\rangle$ and $|n'\rangle$, corresponding to different eigenvalues, must be orthogonal, $\langle n' \mid n\rangle \sim \delta_{n',n}$, since $\hat{H}$ is Hermitian and none of its eigenstates is degenerate.

Moreover, the states $\mid 0\rangle, \mid 1\rangle, \mid 2\rangle, \mid 3\rangle, \ldots, \mid n\rangle, \ldots$ are *simultaneous eigenstates* of $\hat{H}$ and $\hat{N}$; the set $\{\mid n\rangle\}$ constitutes an orthonormal and complete basis:

$$\langle n' \mid n\rangle = \delta_{n',n}, \qquad \sum_{n=0}^{+\infty} \mid n\rangle\langle n \mid = 1. \tag{4.150}$$

4.8.3 Energy Eigenstates in Position Space

Let us now determine the harmonic oscillator wave function in the position representation.

Equations (4.146) to (4.149) show that, knowing the ground state wave function, we can determine any other eigenstate by successive applications of the operator $a^\dagger$ on the ground state. So let us first determine the ground state wave function in the position representation.

The operator $\hat{p}$, defined by $\hat{p} = \hat{P}/\sqrt{m\hbar\omega}$, is given in the position space by

$$\hat{p} = -\frac{i\hbar}{\sqrt{m\hbar\omega}}\frac{d}{dx} = -ix_0\frac{d}{dx}, \tag{4.151}$$

where, as mentioned above, $x_0 = \sqrt{\hbar/(m\omega)}$ is a constant that has the dimensions of length; it sets the length scale of the oscillator. We can easily show that the annihilation and creation operators $\hat{a}$ and $\hat{a}^\dagger$, defined in (4.122), can be written in the position representation as

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\frac{\hat{X}}{x_0} + x_0\frac{d}{dx}\right) = \frac{1}{\sqrt{2}x_0}\left(\hat{X} + x_0^2\frac{d}{dx}\right), \tag{4.152}$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\frac{\hat{X}}{x_0} - x_0\frac{d}{dx}\right) = \frac{1}{\sqrt{2}x_0}\left(\hat{X} - x_0^2\frac{d}{dx}\right). \tag{4.153}$$

Using (4.152) we can write the equation $\hat{a} \mid 0\rangle = 0$ in the position space as

$$\langle x|\hat{a} \mid 0\rangle = \frac{1}{\sqrt{2}x_0}\langle x|\hat{X} + x_0^2\frac{d}{dx} \mid 0\rangle = \frac{1}{\sqrt{2}x_0}\left(x\,\psi_0(x) + x_0^2\frac{d\psi_0(x)}{dx}\right) = 0; \tag{4.154}$$

hence

$$\frac{d\psi_0(x)}{dx} = -\frac{x}{x_0^2}\psi_0(x), \tag{4.155}$$

where $\psi_0(x) = \langle x \mid 0\rangle$ represents the ground state wave function. The solution of this differential equation is

$$\psi_0(x) = A\exp\left(-\frac{x^2}{2x_0^2}\right), \tag{4.156}$$

where A is a constant that can be determined from the normalization condition

$$1 = \int_{-\infty}^{+\infty} dx\,|\psi_0(x)|^2 = A^2\int_{-\infty}^{+\infty} dx\exp\left(-\frac{x^2}{x_0^2}\right) = A^2\sqrt{\pi}x_0; \tag{4.157}$$

hence $A = (m\omega/(\pi\hbar))^{1/4} = 1/\sqrt{\sqrt{\pi}x_0}$. The normalized ground state wave function is then given by

$$\boxed{\psi_0(x) = \frac{1}{\sqrt{\sqrt{\pi}x_0}} \exp\left(-\frac{x^2}{2x_0^2}\right).} \tag{4.158}$$

This is a Gaussian function.

We can then obtain the wave function of any excited state by a series of applications of $\hat{a}^\dagger$ on the ground state. For instance, the first excited state is obtained by one single application of the operator $\hat{a}^\dagger$ of (4.153) on the ground state:

$$\begin{aligned} \langle x \mid 1\rangle &= \langle x|\hat{a}^\dagger \mid 0\rangle = \frac{1}{\sqrt{2}x_0}\left(x - x_0^2\frac{d}{dx}\right)\langle x \mid 0\rangle \\ &= \frac{1}{\sqrt{2}x_0}\left(x - x_0^2\left(-\frac{x}{x_0^2}\right)\right)\psi_0(x) = \frac{\sqrt{2}}{x_0}x\,\psi_0(x) \end{aligned} \tag{4.159}$$

or

$$\psi_1(x) = \frac{\sqrt{2}}{x_0}x\,\psi_0(x) = \sqrt{\frac{2}{\sqrt{\pi}x_0^3}}x\exp\left(-\frac{x^2}{2x_0^2}\right). \tag{4.160}$$

As for the eigenstates of the second and third excited states, we can obtain them by applying $\hat{a}^\dagger$ on the ground state twice and three times, respectively:

$$\langle x \mid 2\rangle = \frac{1}{\sqrt{2!}}\langle x|\left(a^\dagger\right)^2 \mid 0\rangle = \frac{1}{\sqrt{2!}}\left(\frac{1}{\sqrt{2}x_0}\right)^2\left(x - x_0^2\frac{d}{dx}\right)^2\psi_0(x), \tag{4.161}$$

$$\langle x \mid 3\rangle = \frac{1}{\sqrt{3!}}\langle x|\left(a^\dagger\right)^3 \mid 0\rangle = \frac{1}{\sqrt{3!}}\left(\frac{1}{\sqrt{2}x_0}\right)^3\left(x - x_0^2\frac{d}{dx}\right)^3\psi_0(x) \tag{4.162}$$

or

$$\psi_2(x) = \frac{1}{\sqrt{2\sqrt{\pi}x_0}}\left(\frac{2x^2}{x_0^2} - 1\right)\exp\left(-\frac{x^2}{2x_0^2}\right), \quad \psi_3(x) = \frac{1}{\sqrt{3\sqrt{\pi}x_0}}\left(\frac{2x^3}{x_0^3} - \frac{3x}{x_0}\right)\exp\left(-\frac{x^2}{2x_0^2}\right). \tag{4.163}$$

Similarly, using (4.149), (4.153), and (4.158), we can easily infer the energy eigenstate for the nth excited state:

$$\langle x \mid n\rangle = \frac{1}{\sqrt{n!}}\langle x|\left(a^\dagger\right)^n \mid 0\rangle = \frac{1}{\sqrt{n!}}\left(\frac{1}{\sqrt{2}x_0}\right)^n\left(x - x_0^2\frac{d}{dx}\right)^n\psi_0(x), \tag{4.164}$$

which in turn can be rewritten as

$$\boxed{\psi_n(x) = \frac{1}{\sqrt{\sqrt{\pi}2^n n!}}\frac{1}{x_0^{n+1/2}}\left(x - x_0^2\frac{d}{dx}\right)^n\exp\left(-\frac{x^2}{2x_0^2}\right).} \tag{4.165}$$

In summary, by successive applications of $\hat{a}^\dagger = (\hat{X} - x_0^2 d/dx)/(\sqrt{2}x_0)$ on $\psi_0(x)$, we can find the wave function of any excited state $\psi_n(x)$.

Oscillator wave functions and the Hermite polynomials

At this level, we can show that the wave function (4.165) derived from the algebraic method is similar to the one obtained from the first method (4.118). To see this, we simply need to use the following operator identity:

$$e^{-x^2/2}\left(x-\frac{d}{dx}\right)e^{x^2/2}=-\frac{d}{dx}\quad\text{or}\quad e^{-x^2/2x_0^2}\left(x-x_0^2\frac{d}{dx}\right)e^{x^2/2x_0^2}=-x_0^2\frac{d}{dx}. \tag{4.166}$$

An application of this operator n times leads at once to

$$e^{-x^2/2x_0^2}\left(x-x_0^2\frac{d}{dx}\right)^n e^{x^2/2x_0^2}=(-1)^n(x_0^2)^n\frac{d^n}{dx^n}, \tag{4.167}$$

which can be shown to yield

$$\left(x-x_0^2\frac{d}{dx}\right)^n e^{-x^2/2x_0^2}=(-1)^n(x_0^2)^n e^{x^2/2x_0^2}\frac{d^n}{dx^n}e^{-x^2/x_0^2}. \tag{4.168}$$

We can now rewrite the right-hand side of this equation as follows:

$$\begin{aligned}(-1)^n(x_0^2)^n e^{x^2/2x_0^2}\frac{d^n}{dx^n}e^{-x^2/x_0^2} &= x_0^n e^{-x^2/2x_0^2}\left[(-1)^n e^{x^2/x_0^2}\frac{d^n}{d(x/x_0)^n}e^{-x^2/x_0^2}\right]\\ &= x_0^n e^{-x^2/2x_0^2}\left[(-1)^n e^{y^2}\frac{d^n}{dy^n}e^{-y^2}\right]\\ &= x_0^n e^{-x^2/2x_0^2}H_n(y),\end{aligned} \tag{4.169}$$

where $y=x/x_0$ and where $H_n(y)$ are the Hermite polynomials listed in (4.119):

$$H_n(y)=(-1)^n e^{y^2}\frac{d^n}{dy^n}e^{-y^2}. \tag{4.170}$$

Note that the polynomials $H_{2n}(y)$ are even and $H_{2n+1}(y)$ are odd, since $H_n(-y)=(-1)^n H_n(y)$.

Inserting (4.169) into (4.168), we obtain

$$\left(x-x_0^2\frac{d}{dx}\right)^n e^{-x^2/2x_0^2}=x_0^n e^{-x^2/2x_0^2}H_n\left(\frac{x}{x_0}\right); \tag{4.171}$$

substituting this equation into (4.165), we can write the oscillator wave function in terms of the Hermite polynomials as follows:

$$\boxed{\psi_n(x)=\frac{1}{\sqrt{\sqrt{\pi}2^n n!x_0}}e^{-x^2/2x_0^2}H_n\left(\frac{x}{x_0}\right).} \tag{4.172}$$

This wave function is identical with the one obtained from the first method (see Eq. (4.118)).

Remark

This wave function is either even or odd depending on n; in fact, the functions $\psi_{2n}(x)$ are even (i.e., $\psi_{2n}(-x)=\psi_{2n}(x)$) and $\psi_{2n+1}(x)$ are odd (i.e., $\psi_{2n}(-x)=-\psi_{2n}(x)$) since, as can be inferred from Eq (4.120), the Hermite polynomials $H_{2n}(x)$ are even and $H_{2n+1}(x)$ are odd. This is expected because, as mentioned in Section 4.2.4, the wave functions of even one-dimensional potentials have definite parity. Figure 4.9 displays the shapes of the first few wave functions.

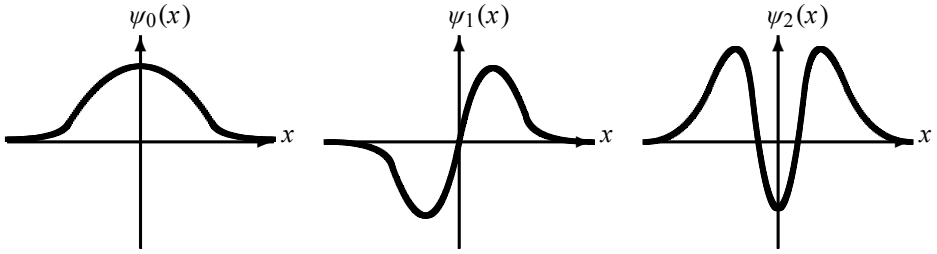


Figure 4.9 Shapes of the first three wave functions of the harmonic oscillator.

4.8.4 The Matrix Representation of Various Operators

Here we look at the matrix representation of several operators in the N-space. In particular, we focus on the representation of the operators $\hat{a}$, $\hat{a}^\dagger$, $\hat{X}$, and $\hat{P}$. First, since the states $|\, n\rangle$ are joint eigenstates of $\hat{H}$ and $\hat{N}$, it is easy to see from (4.130) and (4.132) that $\hat{H}$ and $\hat{N}$ are represented within the $\{|\, n\rangle\}$ basis by infinite diagonal matrices:

$$\langle n'|\hat{N} \mid n\rangle = n\delta_{n',n}, \qquad \langle n'|\hat{H} \mid n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)\delta_{n',n}; \tag{4.173}$$

that is,

$$\hat{N} = \begin{pmatrix} 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 2 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \qquad \hat{H} = \frac{\hbar\omega}{2}\begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 3 & 0 & \cdots \\ 0 & 0 & 5 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{4.174}$$

As for the operators $\hat{a}$, $\hat{a}^\dagger$, $\hat{X}$, $\hat{P}$, none of them are diagonal in the N-representation, since they do not commute with $\hat{N}$. The matrix elements of $\hat{a}$ and $\hat{a}^\dagger$ can be obtained from (4.143) and (4.144):

$$\langle n'|\hat{a} \mid n\rangle = \sqrt{n}\delta_{n',n-1}, \qquad \langle n'|\hat{a}^\dagger \mid n\rangle = \sqrt{n+1}\delta_{n',n+1}; \tag{4.175}$$

that is,

$$\hat{a} = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \qquad \hat{a}^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{4.176}$$

Now, let us find the N-representation of the position and momentum operators, $\hat{X}$ and $\hat{P}$. From (4.122) we can show that $\hat{X}$ and $\hat{P}$ are given in terms of $\hat{a}$ and $\hat{a}^\dagger$ as follows:

$$\hat{X} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^\dagger\right), \qquad \hat{P} = i\sqrt{\frac{m\hbar\omega}{2}}\left(\hat{a}^\dagger - \hat{a}\right). \tag{4.177}$$

Their matrix elements are given by

$$\langle n'|\hat{X} \mid n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}\right), \tag{4.178}$$

$$\langle n'|\hat{P} \mid n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\left(-\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}\right), \tag{4.179}$$

in particular

$$\langle n \mid \hat{X} \mid n\rangle = \langle n \mid \hat{P} \mid n\rangle = 0. \tag{4.180}$$

The matrices corresponding to $\hat{X}$ and $\hat{P}$ are thus given by

$$\hat{X} = \sqrt{\frac{\hbar}{2m\omega}}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \tag{4.181}$$

$$\hat{P} = i\sqrt{\frac{m\hbar\omega}{2}}\begin{pmatrix} 0 & -\sqrt{1} & 0 & 0 & \cdots \\ \sqrt{1} & 0 & -\sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{4.182}$$

As mentioned in Chapter 2, the momentum operator is Hermitian, but not equal to its own complex conjugate: (4.182) shows that $\hat{P}^\dagger = \hat{P}$ and $\hat{P}^* = -\hat{P}$. As for $\hat{X}$, however, it is both Hermitian and equal to its complex conjugate: from (4.181) we have that $\hat{X}^\dagger = \hat{X}^* = \hat{X}$.

Finally, we should mention that the eigenstates $|n\rangle$ are represented by infinite column matrices; the first few states can be written as

$$|\,0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \qquad |\,1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \qquad |\,2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}, \qquad |\,3\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix}, \ldots. \tag{4.183}$$

The set of states $\{|\,n\rangle\}$ forms indeed a complete and orthonormal basis.

4.8.5 Expectation Values of Various Operators

Let us evaluate the expectation values for $\hat{X}^2$ and $\hat{P}^2$ in the N-representation:

$$\hat{X}^2 = \frac{\hbar}{2m\omega}\left(\hat{a}^2 + \hat{a}^{\dagger 2} + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}\right) = \frac{\hbar}{2m\omega}\left(\hat{a}^2 + \hat{a}^{\dagger 2} + 2\hat{a}^\dagger\hat{a} + 1\right), \tag{4.184}$$

$$\hat{P}^2 = -\frac{m\hbar\omega}{2}\left(\hat{a}^2 + \hat{a}^{\dagger 2} - \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}\right) = -\frac{m\hbar\omega}{2}\left(\hat{a}^2 + \hat{a}^{\dagger 2} - 2\hat{a}^\dagger\hat{a} - 1\right), \tag{4.185}$$

where we have used the fact that $\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} = 2\hat{a}^\dagger\hat{a} + 1$. Since the expectation values of $\hat{a}^2$ and $\hat{a}^{\dagger 2}$ are zero, $\langle n \mid \hat{a}^2 \mid n\rangle = \langle n \mid \hat{a}^{\dagger 2} \mid n\rangle = 0$, and $\langle n \mid \hat{a}^\dagger\hat{a} \mid n\rangle = n$, we have

$$\langle n \mid \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} \mid n\rangle = \langle n \mid 2\hat{a}^\dagger\hat{a} + 1 \mid n\rangle = 2n + 1; \tag{4.186}$$

hence

$$\langle n \mid \hat{X}^2 \mid n\rangle = \frac{\hbar}{2m\omega}\langle n \mid \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} \mid n\rangle = \frac{\hbar}{2m\omega}(2n+1), \tag{4.187}$$

$$\langle n \mid \hat{P}^2 \mid n\rangle = \frac{m\hbar\omega}{2}\langle n \mid \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} \mid n\rangle = \frac{m\hbar\omega}{2}(2n+1). \tag{4.188}$$

Comparing (4.187) and (4.188) we see that the expectation values of the potential and kinetic energies are equal and are also equal to half the total energy:

$$\boxed{\frac{m\omega^2}{2}\langle n \mid \hat{X}^2 \mid n\rangle = \frac{1}{2m}\langle n \mid \hat{P}^2 \mid n\rangle = \frac{1}{2}\langle n \mid \hat{H} \mid n\rangle.} \tag{4.189}$$

This result is known as the *Virial theorem*.

We can now easily calculate the product $\Delta x\,\Delta p$ from (4.187) and (4.188). Since $\langle\hat{X}\rangle = \langle\hat{P}\rangle = 0$ we have

$$\Delta x = \sqrt{\langle\hat{X}^2\rangle - \langle\hat{X}\rangle^2} = \sqrt{\langle\hat{X}^2\rangle} = \sqrt{\frac{\hbar}{2m\omega}(2n+1)}, \tag{4.190}$$

$$\Delta p = \sqrt{\langle\hat{P}^2\rangle - \langle\hat{P}\rangle^2} = \sqrt{\langle\hat{P}^2\rangle} = \sqrt{\frac{m\hbar\omega}{2}(2n+1)}; \tag{4.191}$$

hence

$$\Delta x\,\Delta p = \left(n + \frac{1}{2}\right)\hbar \quad\Longrightarrow\quad \Delta x\,\Delta p \geq \frac{\hbar}{2}, \tag{4.192}$$

since $n \geq 0$; this is the Heisenberg uncertainty principle.

4.9 Numerical Solution of the Schrödinger Equation

In this section we are going to show how to solve a one-dimensional Schrödinger equation numerically. The numerical solutions provide an idea about the properties of stationary states.

4.9.1 Numerical Procedure

We want to solve the following equation numerically:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x) \Longrightarrow \frac{d^2\psi}{dx^2} + k^2\psi(x) = 0, \tag{4.193}$$

where $k^2 = 2m[E - V(x)]/\hbar^2$.

First, divide the x-axis into a set of equidistant points with a spacing of $h_0 = \Delta x$, as shown in Figure 4.10a. The wave function $\psi(x)$ can be approximately described by its values at the

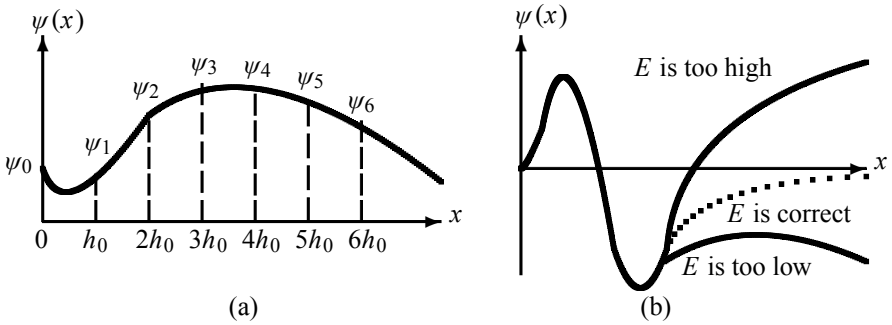


Figure 4.10 (a) Discretization of the wave function. (b) If the energy E used in the computation is too high (too low), the wave function will diverge as $x \to \pm\infty$; but at the appropriate value of E, the wave function converges to the correct values.

points of the grid (i.e., $\psi_0 = \psi(x = 0)$, $\psi_1 = \psi(h_0)$, $\psi_2 = \psi(2h_0)$, $\psi_3 = \psi(3h_0)$, and so on). The first derivative of ψ can then be approximated by

$$\frac{d\psi}{dx} \approx \frac{\psi_{n+1} - \psi_n}{h_0}. \tag{4.194}$$

An analogous approximation for the second derivative is actually a bit tricky. There are several methods to calculate it, but a very efficient procedure is called the *Numerov algorithm* (which is described in standard numerical analysis textbooks). In short, the second derivative is approximated by the so-called three-point difference formula:

$$\frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{h_0^2} = \psi_n'' + \frac{h_0^2}{12}\psi_n'''' + 0(h_0^4). \tag{4.195}$$

From (4.193) we have

$$\psi_n'''' = \frac{d^2}{dx^2}(-k^2\psi)\bigg|_{x=x_n} = -\frac{(k^2\psi)_{n+1} - 2(k^2\psi)_n + (k^2\psi)_{n-1}}{h_0^2}. \tag{4.196}$$

Using $\psi_n'' = -k_n^2\psi_n$ and substituting (4.196) into (4.195) we can show that

$$\psi_{n+1} = \frac{2\left(1 - \frac{5}{12}h_0^2k_n^2\right)\psi_n - \left(1 + \frac{1}{12}h_0^2k_{n-1}^2\right)\psi_{n-1}}{1 + \frac{1}{12}h_0^2k_{n+1}^2}. \tag{4.197}$$

We can thus assign arbitrary values for ψ_0 and ψ_1; this is equivalent to providing the starting (or initial) values for $\psi(x)$ and $\psi'(x)$. Knowing ψ_0 and ψ_1, we can use (4.197) to calculate ψ_2, then ψ_3, then ψ_4, and so on. The solution of a linear equation, equation (4.197), for either ψ_{n+1} or ψ_{n-1} yields a recursion relation for integrating either *forward* or *backward* in x with a local error $O(h_0^6)$. In this way, the solution depends on two arbitrary constants, ψ_0 and ψ_1, as it should for any second-order differential equation (i.e., there are two linearly independent solutions).

The *boundary conditions* play a crucial role in solving any Schrödinger equation. Every boundary condition gives a linear homogeneous equation satisfied by the wave function or its

derivative. For example, in the case of the infinite square well potential and the harmonic oscillator, the conditions $\psi(x_{min}) = 0$, $\psi(x_{max}) = 0$ are satisfied as follows:

- Infinite square well: $\psi(-a/2) = \psi(a/2) = 0$
- Harmonic oscillator: $\psi(-\infty) = \psi(+\infty) = 0$

4.9.2 Algorithm

To solve the Schrödinger equation with the boundary conditions $\psi(x_{min}) = \psi(x_{max}) = 0$, you may proceed as follows. Suppose you want to find the wave function, $\psi^{(n)}(x)$, and the energy E_n for the nth excited[4] state of a system:

- Take $\psi_0 = 0$ and choose ψ_1 (any small number you like), because the value of ψ_1 must be very close to that of ψ_0.
- Choose a *trial* energy E_n.
- With this value of the energy, E_n, together with ψ_0 and ψ_1, you can calculate iteratively the wave function at different values of x; that is, you can calculate ψ_2, ψ_3, ψ_4, ... How? You need simply to inject $\psi_0 = 0$, ψ_1, and E_n into (4.197) and proceed incrementally to calculate ψ_2; then use ψ_1 and ψ_2 to calculate ψ_3; then use ψ_2 and ψ_3 to calculate ψ_4; and so on till you end up with the value of the wave function at $x_n = nh_0$, $\psi_n = \psi(nh_0)$.
- Next, you need to check whether the ψ_n you obtained is zero or not. If ψ_n is zero, this means that you have made the right choice for the trial energy. This value E_n can then be taken as a possible eigenenergy for the system; at this value of E_n, the wave function converges to the correct value (dotted curve in Figure 4.10b). Of course, it is highly unlikely to have chosen the correct energy from a first trial. In this case you need to proceed as follows. If the value of ψ_n obtained is a nonzero positive number or if it diverges, this means that the trial E_n you started with is larger than the correct eigenvalue (Figure 4.10b); on the other hand, if ψ_n is a negative nonzero number, this means that the E_n you started with is less than the true energy. If the ψ_n you end up with is a positive nonzero number, you need to start all over again with a smaller value of the energy. But if the ψ_n you end up with is negative, you need to start again with a larger value of E. You can continue in this way, improving every time, till you end up with a zero value for ψ_n. Note that in practice there is no way to get ψ_n exactly equal to zero. You may stop the procedure the moment ψ_n is sufficiently small; that is, you stop the iteration at the desired accuracy, say at 10^{-8} of its maximum value.

Example 4.3 (Numerical solution of the Schrödinger equation)
A proton is subject to a harmonic oscillator potential $V(x) = m\omega^2 x^2/2$, $\omega = 5.34 \times 10^{21} s^{-1}$.

(a) Find the exact energies of the five lowest states (express them in MeV).

(b) Solve the Schrödinger equation *numerically* and find the energies of the five lowest states and compare them with the exact results obtained in (a). Note: You may use these quantities: rest mass energy of the proton $mc^2 \simeq 10^3$ MeV, $\hbar c \simeq 200\,\text{MeV fm}$, and $\hbar\omega \simeq 3.5\,\text{MeV}$.

[4] We have denoted here the wave function of the nth excited state by $\psi^{(n)}(x)$ to distinguish it from the value of the wave function at $x_n = nh_0$, $\psi_n = \psi(nh_0)$.

Table 4.1 Exact and numerical energies for the five lowest states of the harmonic oscillator.

n	E_n^{Exact} (MeV)	$E_n^{Numeric}$ (MeV)
0.0	1.750 000	1.749 999 999 795
1.0	5.250 000	5.249 999 998 112
2.0	8.750 000	8.749 999 992 829
3.0	12.250 000	12.249 999 982 320
4.0	15.750 000	15.749 999 967 590

Solution

(a) The exact energies can be calculated at once from $E_n = \hbar\omega(n + \frac{1}{2}) \simeq 3.5(n + \frac{1}{2})$ MeV. The results for the five lowest states are listed in Table 4.1.

(b) To obtain the numerical values, we need simply to make use of the Numerov relation (4.197), where $k_n^2(x) = 2m(E_n - \frac{1}{2}m\omega^2x^2)/\hbar^2$. The numerical values involved here can be calculated as follows:

$$\frac{m^2\omega^2}{\hbar^2} = \frac{(mc^2)^2(\hbar\omega)^2}{(\hbar c)^4} \simeq \frac{(10^3\,\text{MeV})^2(3.5\,\text{MeV})^2}{(200\,\text{MeV fm})^4} = 7.66 \times 10^{-4}\,\text{fm}^{-3}, \quad (4.198)$$

$$\frac{2m}{\hbar^2} = \frac{2mc^2}{(\hbar c)^2} \simeq \frac{2 \times 10^3\,\text{MeV}}{(200\,\text{MeV fm})^2} = 0.05\,\text{MeV}^{-1}\,\text{fm}^{-2}. \quad (4.199)$$

The boundary conditions for the harmonic oscillator imply that the wave function vanishes at $x = \pm\infty$, i.e., at $x_{min} = -\infty$ and $x_{max} = \infty$. How does one deal with infinities within a computer program? For this, we need to choose the numerical values of x_{min} and x_{max} in a way that the wave function would not feel the "edge" effects. That is, we simply need to assign numerical values to x_{min} and x_{max} so that they are far away from the turning points $x_{Left} = -\sqrt{2E_n/(m\omega^2)}$ and $x_{Right} = \sqrt{2E_n/(m\omega^2)}$, respectively. For instance, in the case of the ground state, where $E_0 = 1.75$ MeV, we have $x_{Left} = -3.38$ fm and $x_{Right} = 3.38$ fm; we may then take $x_{min} = -20$ fm and $x_{max} = 20$ fm. The wave function should be practically zero at $x = \pm 20$ fm.

To calculate the energies numerically for the five lowest states, a C++ computer code has been prepared (see Appendix C). The numerical results generated by this code are listed in Table 4.1; they are in excellent agreement with the exact results. Figure 4.11 displays the wave functions obtained from this code for the five lowest states for the proton moving in a harmonic oscillator potential (these plotted wave functions are normalized).

4.10 Solved Problems

Problem 4.1

A particle moving in one dimension is in a stationary state whose wave function

$$\psi(x) = \begin{cases} 0, & x < -a, \\ A(1 + \cos\frac{\pi x}{a}), & -a \le x \le a, \\ 0, & x > a, \end{cases}$$

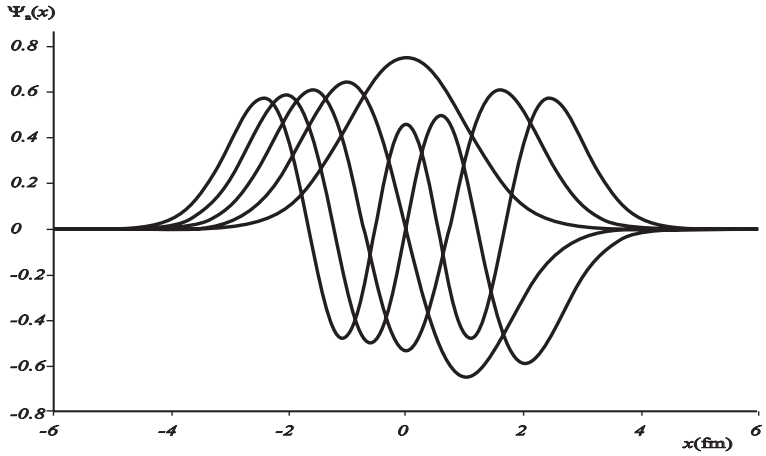


Figure 4.11 Wave functions $\psi_n(x)$ of the five lowest states of a harmonic oscillator potential in terms of x, where the x-axis values are in fm (obtained from the C++ code of Appendix C).

where A and a are real constants.

(a) Is this a physically acceptable wave function? Explain.

(b) Find the magnitude of A so that $\psi(x)$ is normalized.

(c) Evaluate Δx and Δp. Verify that $\Delta x\,\Delta p \geq \hbar/2$.

(d) Find the classically allowed region.

Solution

(a) Since $\psi(x)$ is square integrable, single-valued, continuous, and has a continuous first derivative, it is indeed physically acceptable.

(b) Normalization of $\psi(x)$: using the relation $\cos^2 y = (1+\cos 2y)/2$, we have

$$\begin{aligned} 1 &= \int_{-\infty}^{+\infty} |\psi(x)|^2 dx = A^2 \int_{-a}^{a} dx \left[1 + 2\cos\frac{\pi x}{a} + \cos^2\left(\frac{\pi x}{a}\right)\right] \\ &= A^2 \int_{-a}^{a} dx \left[\frac{3}{2} + 2\cos\frac{\pi x}{a} + \frac{1}{2}\cos\frac{2\pi x}{a}\right] \\ &= \frac{3}{2}A^2 \int_{-a}^{a} dx = 3aA^2; \end{aligned} \tag{4.200}$$

hence $A = 1/\sqrt{3a}$.

(c) As $\psi(x)$ is even, we have $\langle \hat{X} \rangle = \int_{-a}^{+a} \psi^*(x) x \psi(x)\, dx = 0$, since the symmetric integral of an odd function (i.e., $\psi^*(x) x \psi(x)$ is odd) is zero. On the other hand, we also have $\langle \hat{P} \rangle = 0$ because $\psi(x)$ is real and even. We can thus write

$$\Delta x = \sqrt{\langle \hat{X}^2 \rangle}, \qquad \Delta p = \sqrt{\langle \hat{P}^2 \rangle}, \tag{4.201}$$

since $\Delta A = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$. The calculations of $\langle \hat{X}^2 \rangle$ and $\langle \hat{P}^2 \rangle$ are straightforward:

$$\langle \hat{X}^2 \rangle = -\hbar^2 \int_{-a}^{a} \psi^*(x) x^2 \psi(x)\, dx = \frac{1}{3a} \int_{-a}^{a} \left[x^2 + 2x^2 \cos\left(\frac{\pi x}{a}\right) + x^2 \cos^2\left(\frac{\pi x}{a}\right)\right] dx$$

$$= \frac{a^2}{6\pi^2}\left(2\pi^2 - 15\right), \tag{4.202}$$

$$\begin{aligned}\langle \hat{P}^2 \rangle &= -\hbar^2 \int_{-a}^{+a} \psi(x) \frac{d^2\psi(x)}{dx^2}\, dx = \frac{\pi^2\hbar^2}{a^2} A^2 \int_{-a}^{a} \left[\cos\frac{\pi x}{a} + cos^2\left(\frac{\pi x}{a}\right)\right] dx \\ &= \frac{\pi^2\hbar^2}{3a^3} \int_{-a}^{a} \left[\frac{1}{2} + \cos\frac{\pi x}{a} + \frac{1}{2}\cos\frac{2\pi x}{a}\right] dx = \frac{\pi^2\hbar^2}{3a^2}; \end{aligned} \tag{4.203}$$

hence $\Delta x = a\sqrt{1/3 - 5/(2\pi^2)}$ and $\Delta p = \pi\hbar/(\sqrt{3}a)$. We see that the uncertainties product

$$\Delta x\, \Delta p = \frac{\pi\hbar}{3}\sqrt{1 - \frac{15}{2\pi^2}} \tag{4.204}$$

satisfies Heisenberg's uncertainty principle, $\Delta x\, \Delta p > \hbar/2$.

(d) Since $d\psi^2/dx^2$ is zero at the inflection points, we have

$$\frac{d^2\psi}{dx^2} = -\frac{\pi^2}{a^2} A \cos\frac{\pi x}{a} = 0. \tag{4.205}$$

This relation holds when $x = \pm a/2$; hence the classically allowed region is defined by the interval between the inflection points $-a/2 \le x \le a/2$. That is, since $\psi(x)$ decays exponentially for $x > a/2$ and for $x < -a/2$, the energy of the system must be smaller than the potential. Classically, the system cannot be found in this region.

Problem 4.2

Consider a particle of mass m moving freely between $x = 0$ and $x = a$ inside an infinite square well potential.

(a) Calculate the expectation values $\langle \hat{X} \rangle_n$, $\langle \hat{P} \rangle_n$, $\langle \hat{X}^2 \rangle_n$, and $\langle \hat{P}^2 \rangle_n$, and compare them with their classical counterparts.

(b) Calculate the uncertainties product $\Delta x_n\, \Delta p_n$.

(c) Use the result of (b) to estimate the zero-point energy.

Solution

(a) Since $\psi_n(x) = \sqrt{2/a}\sin(n\pi x/a)$ and since it is a real function, we have $\langle \psi_n | \hat{P} | \psi_n \rangle = 0$ because for any real function $\phi(x)$ the integral $\langle \hat{P} \rangle = -i\hbar \int \phi^*(x)(d\phi(x)/dx)\, dx$ is imaginary and this contradicts the fact that $\langle \hat{P} \rangle$ has to be real. On the other hand, the expectation values of $\hat{X}$, $\hat{X}^2$, and $\hat{P}^2$ are

$$\begin{aligned}\langle \psi_n | \hat{X} | \psi_n \rangle &= \int_0^a \psi_n^*(x)\, x\, \psi_n(x)\, dx = \frac{2}{a}\int_0^a x \sin^2\left(\frac{n\pi x}{a}\right) dx \\ &= \frac{1}{a}\int_0^a x\left[1 - \cos\left(\frac{2n\pi x}{a}\right)\right] dx = \frac{a}{2}, \end{aligned} \tag{4.206}$$

$$\begin{aligned}\langle \psi_n | \hat{X}^2 | \psi_n \rangle &= \frac{2}{a}\int_0^a x^2 \sin^2\left(\frac{n\pi x}{a}\right) dx = \frac{1}{a}\int_0^a x^2\left[1 - \cos\left(\frac{2n\pi x}{a}\right)\right] dx \\ &= \frac{a^2}{3} - \frac{1}{a}\int_0^a x^2 \cos\left(\frac{2n\pi x}{a}\right) dx \end{aligned}$$

$$= \frac{a^2}{3} - \frac{1}{2n\pi}x^2 \sin\left(\frac{2n\pi x}{a}\right)\Big|_{x=0}^{x=a} + \frac{1}{n\pi}\int_0^a x \sin\left(\frac{2n\pi x}{a}\right) dx$$

$$= \frac{a^2}{3} - \frac{a^2}{2n^2\pi^2}, \tag{4.207}$$

$$\langle\psi_n|\hat{P}^2|\psi_n\rangle = -\hbar^2\int_0^a \psi_n^*(x)\frac{d^2\psi_n(x)}{dx^2}dx = \frac{n^2\pi^2\hbar^2}{a^2}\int_0^a |\psi_n(x)|^2 dx = \frac{n^2\pi^2\hbar^2}{a^2}. \tag{4.208}$$

In deriving the previous three expressions, we have used integrations by parts. Since $E_n = n^2\pi^2\hbar^2/(2ma^2)$, we may write

$$\langle\psi_n|\hat{P}^2|\psi_n\rangle = \frac{n^2\pi^2\hbar^2}{a^2} = 2mE_n. \tag{4.209}$$

To calculate the classical average values x_{av}, p_{av}, x_{av}^2, p_{av}^2, it is easy first to infer that $p_{av} = 0$ and $p_{av}^2 = 2mE$, since the particle moves to the right with *constant* momentum $p = mv$ and to the left with $p = -mv$. As the particle moves at constant speed, we have $x = vt$, hence

$$x_{av} = \frac{1}{T}\int_0^T x(t)\,dt = \frac{v}{T}\int_0^T t\,dt = v\frac{T}{2} = \frac{a}{2}, \tag{4.210}$$

$$x_{av}^2 = \frac{1}{T}\int_0^T x^2(t)\,dt = \frac{v^2}{T}\int_0^T t^2 dt = \frac{1}{3}v^2T^2 = \frac{a^2}{3}, \tag{4.211}$$

where T is half[5] of the period of the motion, with $a = vT$.

We conclude that, while the average classical and quantum expressions for x, p and p^2 are identical, a comparison of (4.207) and (4.211) yields

$$\langle\psi_n|\hat{X}^2|\psi_n\rangle = \frac{a^2}{3} - \frac{a^2}{2n^2\pi^2} = x_{av}^2 - \frac{a^2}{2n^2\pi^2}, \tag{4.212}$$

so that in the limit of large quantum numbers, the quantum expression $\langle\psi_n|\hat{X}^2|\psi_n\rangle$ matches with its classical counterpart x_{av}^2: $\lim_{n\longrightarrow\infty}\langle\psi_n|\hat{X}^2|\psi_n\rangle = a^2/3 = x_{av}^2$.

(b) The position and the momentum uncertainties can be calculated from (4.206) to (4.208):

$$\Delta x_n = \sqrt{\langle\psi_n|\hat{X}^2|\psi_n\rangle - \langle\psi_n|\hat{X}|\psi_n\rangle^2} = \sqrt{\frac{a^2}{3} - \frac{a^2}{2n^2\pi^2} - \frac{a^2}{4}} = a\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}}, \tag{4.213}$$

$$\Delta p_n = \sqrt{\langle\psi_n|\hat{P}^2|\psi_n\rangle - \langle\psi_n|\hat{P}|\psi_n\rangle^2} = \sqrt{\langle\psi_n|\hat{P}^2|\psi_n\rangle} = \frac{n\pi\hbar}{a}, \tag{4.214}$$

hence

$$\Delta x_n\,\Delta p_n = n\pi\hbar\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}}. \tag{4.215}$$

(c) Equation (4.214) shows that the momentum uncertainty for the ground state is not zero, but

$$\Delta p_1 = \frac{\pi\hbar}{a}. \tag{4.216}$$

[5] We may parameterize the other half of the motion by $x = -vt$, which when inserted in (4.210) and (4.211), where the variable t varies between $-T$ and 0, the integrals would yield the same results, namely $x_{av} = a/2$ and $x_{av}^2 = a^2/3$, respectively.

This leads to a nonzero kinetic energy. Therefore, the lowest value of the particle's kinetic energy is of the order of $E_{min} \sim (\Delta p_1)^2/(2m) \sim \pi^2\hbar^2/(2ma^2)$. This value, which is in full agreement with the ground state energy, $E_1 = \pi^2\hbar^2/(2ma^2)$, is the zero-point energy of the particle.

Problem 4.3
An electron is moving freely inside a one-dimensional infinite potential box with walls at $x = 0$ and $x = a$. If the electron is initially in the ground state ($n = 1$) of the box and if we *suddenly* quadruple the size of the box (i.e., the right-hand side wall is moved instantaneously from $x = a$ to $x = 4a$), calculate the probability of finding the electron in:

(a) the ground state of the new box and

(b) the first excited state of the new box.

Solution
Initially, the electron is in the ground state of the box $x = 0$ and $x = a$; its energy and wave function are

$$E_1 = \frac{\pi^2\hbar^2}{2ma^2}, \qquad \phi_1(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right). \tag{4.217}$$

(a) Once in the new box, $x = 0$ and $x = 4a$, the ground state energy and wave function of the electron are

$$E_1' = \frac{\pi^2\hbar^2}{2m(4a)^2} = \frac{\pi^2\hbar^2}{32ma^2}, \qquad \psi_1(x) = \frac{1}{\sqrt{2a}} \sin\left(\frac{\pi x}{4a}\right). \tag{4.218}$$

The probability of finding the electron in $\psi_1(x)$ is

$$P(E_1') = |\langle\psi_1|\phi_1\rangle|^2 = \left|\int_0^a \psi_1^*(x)\phi_1(x)dx\right|^2 = \frac{1}{a^2}\left|\int_0^a \sin\left(\frac{\pi x}{4a}\right)\sin\left(\frac{\pi x}{a}\right)dx\right|^2; \tag{4.219}$$

the upper limit of the integral sign is a (and not $4a$) because $\phi_1(x)$ is limited to the region between 0 and a. Using the relation $\sin a \sin b = \frac{1}{2}\cos(a - b) - \frac{1}{2}\cos(a + b)$, we have $\sin(\pi x/4a)\sin(\pi x/a) = \frac{1}{2}\cos(3\pi x/4a) - \frac{1}{2}\cos(5\pi x/4a)$; hence

$$\begin{aligned} P(E_1') &= \frac{1}{a^2}\left|\frac{1}{2}\int_0^a \cos\left(\frac{3\pi x}{4a}\right)dx - \frac{1}{2}\int_0^a \cos\left(\frac{5\pi x}{4a}\right)dx\right|^2 \\ &= \frac{128}{15^2\pi^2} = 0.058 = 5.8\%. \end{aligned} \tag{4.220}$$

(b) If the electron is in the first excited state of the new box, its energy and wave function are

$$E_2' = \frac{\pi^2\hbar^2}{8ma^2}, \qquad \psi_2(x) = \frac{1}{\sqrt{2a}} \sin\left(\frac{\pi x}{2a}\right). \tag{4.221}$$

The corresponding probability is

$$\begin{aligned} P(E_2') &= |\langle\psi_2|\phi_1\rangle|^2 = \left|\int_0^a \psi_2^*(x)\phi_1(x)dx\right|^2 = \frac{1}{a^2}\left|\int_0^a \sin\left(\frac{\pi x}{2a}\right)\sin\left(\frac{\pi x}{a}\right)dx\right|^2 \\ &= \frac{16}{9\pi^2} = 0.18 = 18\%. \end{aligned} \tag{4.222}$$

Problem 4.4

Consider a particle of mass m subject to an attractive delta potential $V(x) = -V_0\,\delta(x)$, where $V_0 > 0$ (V_0 has the dimensions of Energy×Distance).

(a) In the case of negative energies, show that this particle has only one bound state; find the binding energy and the wave function.

(b) Calculate the probability of finding the particle in the interval $-a \leq x \leq a$.

(c) What is the probability that the particle remains bound when V_0 is (i) halved suddenly, (ii) quadrupled suddenly?

(d) Study the scattering case (i.e., $E > 0$) and calculate the reflection and transmission coefficients as a function of the wave number k.

Solution

(a) Let us consider first the bound state case $E < 0$. We can write the Schrödinger equation as follows:

$$\frac{d^2\psi(x)}{dx^2} + \frac{2mV_0}{\hbar^2}\delta(x)\psi(x) + \frac{2mE}{\hbar^2}\psi(x) = 0. \tag{4.223}$$

Since $\delta(x)$ vanishes for $x \neq 0$, this equation becomes

$$\frac{d^2\psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0. \tag{4.224}$$

The bound solutions require that $\psi(x)$ vanishes at $x = \pm\infty$; these bound solutions are given by

$$\psi(x) = \begin{cases} \psi_-(x) = Ae^{kx}, & x < 0, \\ \psi_+(x) = Be^{-kx}, & x > 0, \end{cases} \tag{4.225}$$

where $k = \sqrt{2m|E|}/\hbar$. Since $\psi(x)$ is continuous at $x = 0$, $\psi_-(0) = \psi_+(0)$, we have $A = B$. Thus, the wave function is given by $\psi(x) = Ae^{-k|x|}$; note that $\psi(x)$ is even.

The energy can be obtained from the discontinuity condition of the first derivative of the wave function, which in turn can be obtained by integrating (4.223) from $-\varepsilon$ to $+\varepsilon$,

$$\int_{-\varepsilon}^{+\varepsilon} dx \frac{d^2\psi(x)}{dx^2} + \frac{2mV_0}{\hbar^2}\int_{-\varepsilon}^{+\varepsilon}\delta(x)\psi(x)dx + \frac{2mE}{\hbar^2}\int_{-\varepsilon}^{+\varepsilon}\psi(x)dx = 0, \tag{4.226}$$

and then letting $\varepsilon \to 0$. Using the facts that

$$\int_{-\varepsilon}^{+\varepsilon} dx \frac{d^2\psi(x)}{dx^2} = \left.\frac{d\psi(x)}{dx}\right|_{x=+\varepsilon} - \left.\frac{d\psi(x)}{dx}\right|_{x=-\varepsilon} = \left.\frac{d\psi_+(x)}{dx}\right|_{x=+\varepsilon} - \left.\frac{d\psi_-(x)}{dx}\right|_{x=-\varepsilon} \tag{4.227}$$

and that $\int_{-\varepsilon}^{+\varepsilon}\psi(x)dx = 0$ (because $\psi(x)$ is even), we can rewrite (4.226) as follows:

$$\lim_{\varepsilon\to 0}\left(\left.\frac{d\psi_+(x)}{dx}\right|_{x=+\varepsilon} - \left.\frac{d\psi_-(x)}{dx}\right|_{x=-\varepsilon}\right)_{\varepsilon=0} + \frac{2mV_0}{\hbar^2}\psi(0) = 0, \tag{4.228}$$

since the wave function is continuous at $x = 0$, but its first derivative is not. Substituting (4.225) into (4.228) and using $A = B$, we obtain

$$(-2kA) + \frac{2mV_0}{\hbar^2}A = 0 \tag{4.229}$$

or $k = mV_0/\hbar^2$. But since $k = \sqrt{2m|E|/\hbar^2}$, we have $mV_0/\hbar^2 = \sqrt{2m|E|/\hbar^2}$, and since the energy is negative, we conclude that $E = -mV_0^2/(2\hbar^2)$. There is, therefore, only one bound state solution. As for the excited states, all of them are unbound. We may normalize $\psi(x)$,

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} \psi^*(x)\psi(x)\,dx = A^2 \int_{-\infty}^{0} \exp(2kx)\,dx + A^2 \int_{0}^{\infty} \exp(-2kx)\,dx \\ &= 2A^2 \int_0^{\infty} \exp(-2kx)\,dx = \frac{A^2}{k}, \end{aligned} \tag{4.230}$$

hence $A = \sqrt{k}$. The normalized wave function is thus given by $\psi(x) = \sqrt{k}e^{-k|x|}$. So the energy and normalized wave function of the bound state are given by

$$E = -\frac{mV_0^2}{2\hbar^2}, \qquad \psi(x) = \sqrt{\frac{mV_0}{\hbar^2}} \exp\left(-\frac{mV_0}{\hbar^2}|x|\right). \tag{4.231}$$

(b) Since the wave function $\psi(x) = \sqrt{k}e^{-k|x|}$ is normalized, the probability of finding the particle in the interval $-a \le x \le a$ is given by

$$\begin{aligned} P &= \frac{\int_{-a}^{a} |\psi(x)|^2\,dx}{\int_{-\infty}^{\infty} |\psi(x)|^2\,dx} = \int_{-a}^{a} |\psi(x)|^2\,dx = k\int_{-a}^{a} e^{-2k|x|}dx \\ &= k\int_{-a}^{0} e^{2kx}dx + k\int_{0}^{a} e^{-2kx}dx = 2k\int_{0}^{a} e^{-2kx}dx \\ &= 1 - e^{-2ka} = 1 - e^{-2mV_0a/\hbar^2}. \end{aligned} \tag{4.232}$$

(c) If the strength of the potential changed suddenly from V_0 to V_1, the wave function will be given by $\psi_1(x) = \sqrt{mV_1/\hbar^2}\exp(-mV_1|x|/\hbar^2)$. The probability that the particle remains in the bound state $\psi_1(x)$ is

$$\begin{aligned} P &= |\langle\psi_1|\psi\rangle|^2 = \left|\int_{-\infty}^{\infty} {\psi_1}^*(x)\psi(x)\,dx\right|^2 \\ &= \left|\frac{m}{\hbar^2}\sqrt{V_0V_1}\int_{-\infty}^{\infty} \exp\left(-\frac{m(V_0+V_1)}{\hbar^2}|x|\right)dx\right|^2 \\ &= \left|2\frac{m}{\hbar^2}\sqrt{V_0V_1}\int_{0}^{\infty} \exp\left(-\frac{m(V_0+V_1)}{\hbar^2}x\right)dx\right|^2 = \frac{4V_0V_1}{(V_0+V_1)^2}. \end{aligned} \tag{4.233}$$

(i) In the case where the strength of the potential is halved, $V_1 = \frac{1}{2}V_0$, the probability that the particle remains bound is

$$P = \frac{2V_0^2}{(V_0 + \frac{1}{2}V_0)^2} = \frac{8}{9} = 89\%. \tag{4.234}$$

(ii) When the strength is quadrupled, $V_1 = 4V_0$, the probability is given by

$$P = \frac{16V_0^2}{(5V_0)^2} = \frac{16}{25} = 64\%. \tag{4.235}$$

(d) The case $E > 0$ corresponds to a free motion and the energy levels represent a continuum. The solution of the Schrödinger equation for $E > 0$ is given by

$$\psi(x) = \begin{cases} \psi_-(x) = Ae^{ikx} + Be^{-ikx}, & x < 0, \\ \psi_+(x) = Ce^{ikx}, & x > 0, \end{cases} \tag{4.236}$$

where $k = \sqrt{2mE}/\hbar$; this corresponds to a plane wave incident from the left together with a reflected wave in the region $x < 0$, and only a transmitted wave for $x > 0$.

The values of the constants A and B are to be found from the continuity relations. On the one hand, the continuity of $\psi(x)$ at $x = 0$ yields

$$A + B = C \tag{4.237}$$

and, on the other hand, substituting (4.236) into (4.228), we end up with

$$ik(C - A + B) + \frac{2mV_0}{\hbar^2}C = 0. \tag{4.238}$$

Solving (4.237) and (4.238) for B/A and C/A, we find

$$\frac{B}{A} = \frac{-1}{1 + \frac{ik\hbar^2}{mV_0}}, \qquad \frac{C}{A} = \frac{1}{1 - \frac{imV_0}{\hbar^2 k}}. \tag{4.239}$$

Thus, the reflection and transmission coefficients are

$$R = \left|\frac{B}{A}\right|^2 = \frac{1}{1 + \frac{\hbar^4 k^2}{m^2 V_0^2}} = \frac{1}{1 + \frac{2\hbar^2 E}{mV_0^2}}, \quad T = \left|\frac{C}{A}\right|^2 = \frac{1}{1 + \frac{m^2 V_0^2}{\hbar^4 k^2}} = \frac{1}{1 + \frac{mV_0^2}{2\hbar^2 E}}, \tag{4.240}$$

with $R + T = 1$.

Problem 4.5

A particle of mass m is subject to an attractive double-delta potential $V(x) = -V_0\delta(x - a) - V_0\delta(x + a)$, where $V_0 > 0$. Consider only the case of negative energies.

(a) Obtain the wave functions of the bound states.

(b) Derive the eigenvalue equations.

(c) Specify the number of bound states and the limit on their energies. Is the ground state an even state or an odd state?

(d) Estimate the ground state energy for the limits $a \to 0$ and $a \to \infty$.

Solution

(a) The Schrödinger equation for this problem is

$$\frac{d^2\psi(x)}{dx^2} + \frac{2mV_0}{\hbar^2}\left[\delta(x - a) + \delta(x + a)\right]\psi(x) + \frac{2mE}{\hbar^2}\psi(x) = 0. \tag{4.241}$$

For $x \neq \pm a$ this equation becomes

$$\frac{d^2\psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0 \qquad \text{or} \qquad \frac{d^2\psi(x)}{dx^2} - k^2\psi(x) = 0, \tag{4.242}$$

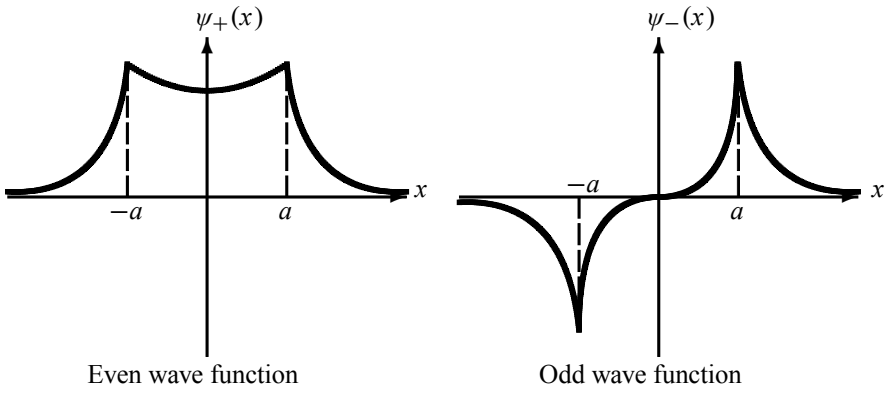


Figure 4.12 Shapes of the even and odd wave functions for $V(x) = -V_0\delta(x-a) - V_0\delta(x+a)$.

where $k^2 = -2mE/\hbar^2 = 2m|E|/\hbar^2$, since this problem deals only with the bound states $E < 0$.

Since the potential is symmetric, $V(-x) = V(x)$, the wave function is either even or odd; we will denote the even states by $\psi_+(x)$ and the odd states by $\psi_-(x)$. The bound state solutions for $E < 0$ require that $\psi_\pm(x)$ vanish at $x = \pm\infty$:

$$\psi_\pm(x) = \begin{cases} Ae^{-kx}, & x > a, \\ \frac{B}{2}\left(e^{kx} \pm e^{-kx}\right), & -a < x < a, \\ \pm Ae^{kx}, & x < -a; \end{cases} \tag{4.243}$$

hence

$$\psi_+(x) = \begin{cases} Ae^{-kx}, \\ B\cosh kx, \\ Ae^{kx}, \end{cases} \qquad \psi_-(x) = \begin{cases} Ae^{-kx}, & x > a, \\ B\sinh kx, & -a < x < a, \\ -Ae^{kx}, & x < -a. \end{cases} \tag{4.244}$$

The shapes of $\psi_\pm(x)$ are displayed in Figure 4.12.

(b) As for the energy eigenvalues, they can be obtained from the boundary conditions. The continuity condition at $x = a$ of $\psi_+(x)$ leads to

$$Ae^{-ka} = B\cosh ka \tag{4.245}$$

and that of $\psi_-(x)$ leads to

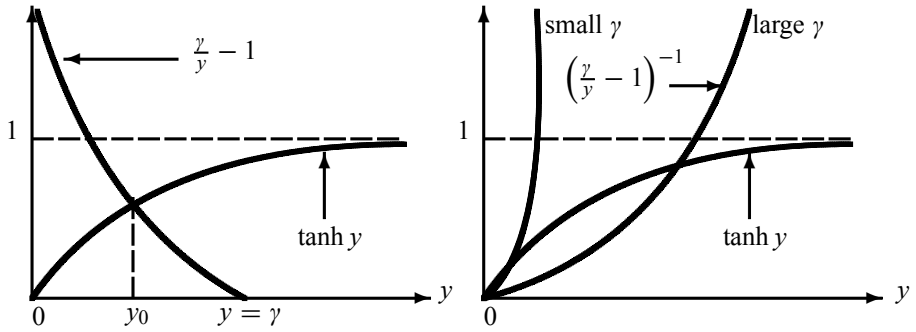
$$Ae^{-ka} = B\sinh ka. \tag{4.246}$$

To obtain the discontinuity condition for the first derivative of $\psi_+(x)$ at $x = a$, we need to integrate (4.241):

$$\lim_{\varepsilon\to 0}\left[\psi'_+(a+\varepsilon) - \psi'_+(a-\varepsilon)\right] + \frac{2mV_0}{\hbar^2}\psi_+(a) = 0; \tag{4.247}$$

hence

$$-kAe^{-ka} - kB\sinh ka + \frac{2mV_0}{\hbar^2}Ae^{-ka} = 0 \implies A\left(\frac{2mV_0}{k\hbar^2} - 1\right)e^{-ka} = B\sinh ka. \tag{4.248}$$



(a) Eigenvalues for even states (b) Eigenvalues for odd states

Figure 4.13 Graphical solutions of the eigenvalue equations for the even states and the odd states for the double-delta potential $V(x) = -V_0\delta(x-a) - V_0\delta(x+a)$.

Similarly, the continuity of the first derivative of $\psi_-(x)$ at $x = a$ yields

$$-kAe^{-ka} - kB\cosh ka + \frac{2mV_0}{\hbar^2}Ae^{-ka} = 0 \implies A\left(\frac{2mV_0}{k\hbar^2} - 1\right)e^{-ka} = B\cosh ka. \tag{4.249}$$

Dividing (4.248) by (4.245) we obtain the eigenvalue equation for the even solutions:

$$\frac{2mV_0}{k\hbar^2} - 1 = \tanh ka \quad \implies \quad \tanh y = \frac{\gamma}{y} - 1, \tag{4.250}$$

where $y = ka$ and $\gamma = 2maV_0/\hbar^2$. The eigenvalue equation for the odd solutions can be obtained by dividing (4.249) by (4.246):

$$\frac{2mV_0}{k\hbar^2} - 1 = \coth ka \quad \implies \quad \coth y = \frac{\gamma}{y} - 1 \quad \implies \quad \tanh y = \left(\frac{\gamma}{y} - 1\right)^{-1}, \tag{4.251}$$

because $\coth y = 1/\tanh y$.

To obtain the energy eigenvalues for the even and odd solutions, we need to solve the transcendental equations (4.250) and (4.251). These equations can be solved graphically. In what follows, let us determine the upper and lower limits of the energy for both the even and odd solutions.

(c) To find the number of bound states and the limits on the energy, let us consider the even and odd states separately.

Energies corresponding to the even solutions

There is only one bound state, since the curves $\tanh y$ and $\gamma/y - 1$ intersect only once (Figure 4.13a); we call this point $y = y_0$. When $y = \gamma$ we have $\gamma/y - 1 = 0$, while $\tanh\gamma > 0$. Therefore $y_0 < \gamma$. On the other hand, since $\tanh y_0 < 1$ we have $\gamma/y_0 - 1 < 1$ or $y_0 > \gamma/2$. We conclude then that $\gamma/2 < y_0 < \gamma$ or

$$\frac{\gamma}{2} < y_0 < \gamma \quad \implies \quad -\frac{2mV_0^2}{\hbar^2} < E_{even} < -\frac{mV_0^2}{2\hbar^2}. \tag{4.252}$$

In deriving this relation, we have used the fact that $\gamma^2/4 < y_0^2 < \gamma^2$ where $\gamma = 2maV_0/\hbar^2$ and $y_0^2 = k_0^2a^2 = -2ma^2E_{even}/\hbar^2$. So there is always one even bound state, the ground state, whose energy lies within the range specified by (4.252).

Energies corresponding to the odd solutions

As shown in Figure 4.13b, if the slope of $(\gamma/y-1)^{-1}$ at $y=0$ is smaller than the slope of $\tanh y$, i.e.,

$$\frac{d}{dy}\left(\frac{\gamma}{y}-1\right)^{-1}\bigg|_{y=0} < \frac{d\tanh y}{dy}\bigg|_{y=0} \quad \Longrightarrow \quad \frac{1}{\gamma}<1 \tag{4.253}$$

or

$$\gamma > 1 \qquad \Longrightarrow \qquad V_0 > \frac{\hbar^2}{2ma}, \tag{4.254}$$

there would be only one bound state because the curves $\tanh y$ and $(\gamma/y-1)^{-1}$ would intersect once. But if $\gamma < 1$ or $V_0 < \hbar^2/(2ma)$, there would be no odd bound states, for the curves of $\tanh y$ and $(\gamma/y-1)^{-1}$ would never intersect.

Note that if $y=\gamma/2$ we have $(\gamma/y-1)^{-1}=1$. Thus the intersection of $\tanh y$ and $(\gamma/y-1)^{-1}$, if it takes place at all, has to take place for $y<\gamma/2$. That is, the odd bound states occur only when

$$y<\frac{\gamma}{2} \qquad \Longrightarrow \qquad E_{odd} > -\frac{mV_0^2}{2\hbar^2}. \tag{4.255}$$

A comparison of (4.252) and (4.255) shows that the energies corresponding to even states are smaller than those of odd states:

$$E_{even} < E_{odd}. \tag{4.256}$$

Thus, the even bound state is the ground state. Using this result, we may infer (a) if $\gamma<1$ there are no odd bound states, but there is always one even bound state, the ground state; (b) if $\gamma>1$ there are two bound states: the ground state (even) and the first excited state (odd).

We may summarize these results as follows:

$$\boxed{\text{If} \quad \gamma<1 \quad \text{or} \quad V_0<\frac{\hbar^2}{2ma} \longrightarrow \text{there is only one bound state.}} \tag{4.257}$$

$$\boxed{\text{If} \quad \gamma>1 \quad \text{or} \quad V_0>\frac{\hbar^2}{2ma} \longrightarrow \text{there are two bound states .}} \tag{4.258}$$

(d) In the limit $a \longrightarrow 0$ we have $y \longrightarrow 0$ and $\gamma \longrightarrow 0$; hence the even transcendental equation $\tanh y = \gamma/y-1$ reduces to $y \simeq \gamma/y-1$ or $y=\gamma$, which in turn leads to $y^2=(ka)^2=\gamma^2$ or $-2ma^2E_{even}/\hbar^2=(2maV_0/\hbar^2)^2$:

$$E_{even}=-\frac{2mV_0^2}{\hbar^2}. \tag{4.259}$$

Note that in the limit $a \longrightarrow 0$, the potential $V(x)=-V_0\delta(x-a)-V_0\delta(x+a)$ reduces to $V(x)=-2V_0\delta(x)$. We can see that the ground state energy (4.231) of the single-delta potential is identical with (4.259) provided we replace V_0 in (4.231) by $2V_0$.

In the limit $a \longrightarrow \infty$, we have $y \longrightarrow \infty$ and $\gamma \longrightarrow \infty$; hence $\tanh y = \gamma/y-1$ reduces to $1 \simeq \gamma/y-1$ or $y=\gamma/2$. This leads to $y^2=(ka)^2=\gamma^2/4$ or $-2ma^2E_{even}/\hbar^2=(maV_0/\hbar^2)^2$:

$$E_{even}=-\frac{mV_0^2}{2\hbar^2}. \tag{4.260}$$

This relation is identical with that of the single-delta potential (4.231).

Problem 4.6
Consider a particle of mass m subject to the potential

$$V(x) = \begin{cases} \infty, & x \leq 0, \\ -V_0\delta(x-a), & x > 0, \end{cases}$$

where $V_0 > 0$. Discuss the existence of bound states in terms of the size of a.

Solution
The Schrödinger equation for $x > 0$ is

$$\frac{d^2\psi(x)}{dx^2} + \left[\frac{2mV_0}{\hbar^2}\delta(x-a) - k^2\right]\psi(x) = 0, \tag{4.261}$$

where $k^2 = -2mE/\hbar^2$, since we are looking here at the bound states only, $E < 0$. The solutions of this equation are

$$\psi(x) = \begin{cases} \psi_1(x) = Ae^{kx} + Be^{-kx}, & 0 < x < a, \\ \psi_2(x) = Ce^{-kx}, & x > a. \end{cases} \tag{4.262}$$

The energy eigenvalues can be obtained from the boundary conditions. As the wave function vanishes at $x = 0$, we have

$$\psi_1(0) = 0 \quad \Longrightarrow \quad A + B = 0 \quad \Longrightarrow \quad B = -A. \tag{4.263}$$

The continuity condition at $x = a$ of $\psi(x)$, $\psi_1(a) = \psi_2(a)$, leads to

$$Ae^{ka} - Ae^{-ka} = Ce^{-ka}. \tag{4.264}$$

To obtain the discontinuity condition for the first derivative of $\psi(x)$ at $x = a$, we need to integrate (4.261):

$$\lim_{\varepsilon\to a}\left[\psi_2'(a+\varepsilon) - \psi_1'(a-\varepsilon)\right] + \frac{2mV_0}{\hbar^2}\psi_2(a) = 0 \tag{4.265}$$

or

$$-kCe^{-ka} - kAe^{ka} - kAe^{-ka} + \frac{2mV_0}{\hbar^2}Ce^{-ka} = 0 \tag{4.266}$$

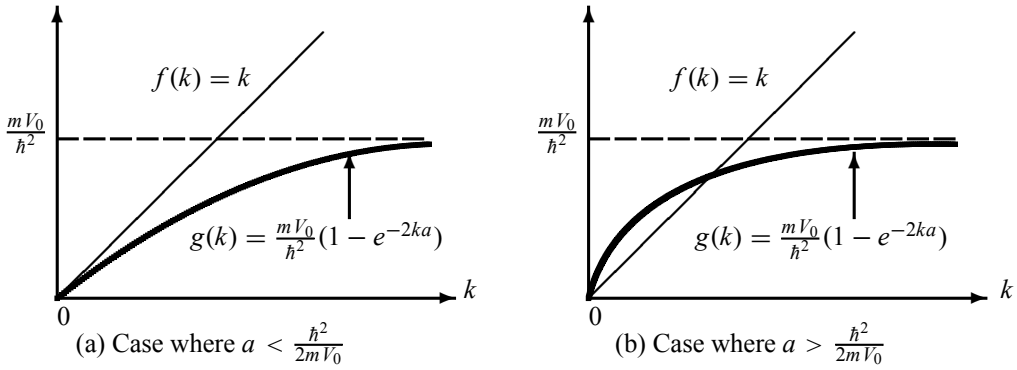
Substituting $Ce^{-ka} = Ae^{ka} - Ae^{-ka}$ or (4.264) into (4.266) we have

$$-kAe^{ka} + kAe^{-ka} - kAe^{ka} - kAe^{-ka} + \frac{2mV_0}{\hbar^2}\left(Ae^{ka} - Ae^{-ka}\right) = 0. \tag{4.267}$$

From this point on, we can proceed in two different, yet equivalent, ways. These two methods differ merely in the way we exploit (4.267). For completeness of the presentation, let us discuss both methods.

First method
The second and fourth terms of (4.267) cancel each other, so we can reduce it to

$$-kAe^{ka} - kAe^{ka} + \frac{2mV_0}{\hbar^2}\left(Ae^{ka} - Ae^{-ka}\right) = 0, \tag{4.268}$$



(a) Case where $a < \frac{\hbar^2}{2mV_0}$ (b) Case where $a > \frac{\hbar^2}{2mV_0}$

Figure 4.14 Graphical solutions of $f(k) = g(k)$ or $k = (mV_0/\hbar^2)(1 - e^{-2ka})$. If the slope of $g(k)$ is smaller than 1, i.e., $a < \hbar^2/(2mV_0)$, no bound state will exist, but if the slope of $g(k)$ is greater than 1, i.e., $a > \frac{\hbar^2}{2mV_0}$, there will be only one bound state.

which in turn leads to the following transcendental equation:

$$k = \frac{mV_0}{\hbar^2}\left(1 - e^{-2ka}\right). \tag{4.269}$$

The energy eigenvalues are given by the intersection of the curves $f(k) = k$ and $g(k) = mV_0(1 - e^{-2ka})/\hbar^2$. As the slope of $f(k)$ is equal to 1, if the slope of $g(k)$ at $k = 0$ is smaller than 1 (i.e., $a < \hbar^2/(2mV_0)$), there will be no bound states (Figure 4.14a). But if the slope of $g(k)$ is greater than 1 (i.e., $a > \hbar^2/(2mV_0)$),

$$\left.\frac{dg(k)}{dk}\right|_{k=0} > 1 \qquad \text{or} \qquad a > \frac{\hbar^2}{2mV_0}, \tag{4.270}$$

and there will be one bound state (Figure 4.14b).

Second method

We simply combine the first and second terms of (4.267) to generate $-2kA\sinh(ka)$; the third and fourth terms yield $-2kA\cosh(ka)$; and the fifth and sixth terms lead to $2A(2mV_0/\hbar^2)\sinh ka$. Hence

$$-2kA\sinh ka - 2kA\cosh ka + (2A)\frac{2mV_0}{\hbar^2}\sinh ka = 0, \tag{4.271}$$

which leads to

$$\gamma\coth\gamma = \frac{2mV_0}{\hbar^2}a - \gamma, \tag{4.272}$$

where $\gamma = ka$. The energy eigenvalues are given by the intersection of the curves $h(\gamma) = \gamma\coth\gamma$ and $u(\gamma) = 2mV_0a/\hbar^2 - \gamma$. As displayed in Figure 4.15a, if $a < 2mV_0/\hbar^2$, no bound state solution will exist, since the curves of $h(\gamma)$ and $u(\gamma)$ do not intersect. But if $a > 2mV_0/\hbar^2$, the curves intersect only once; hence there will be one bound state (Figure 4.15b).

We may summarize the results as follows:

$$a < \frac{\hbar^2}{2mV_0} \quad \Longrightarrow \quad \text{no bound states,} \tag{4.273}$$

$$a > \frac{\hbar^2}{2mV_0} \quad \Longrightarrow \quad \text{one bound state.} \tag{4.274}$$

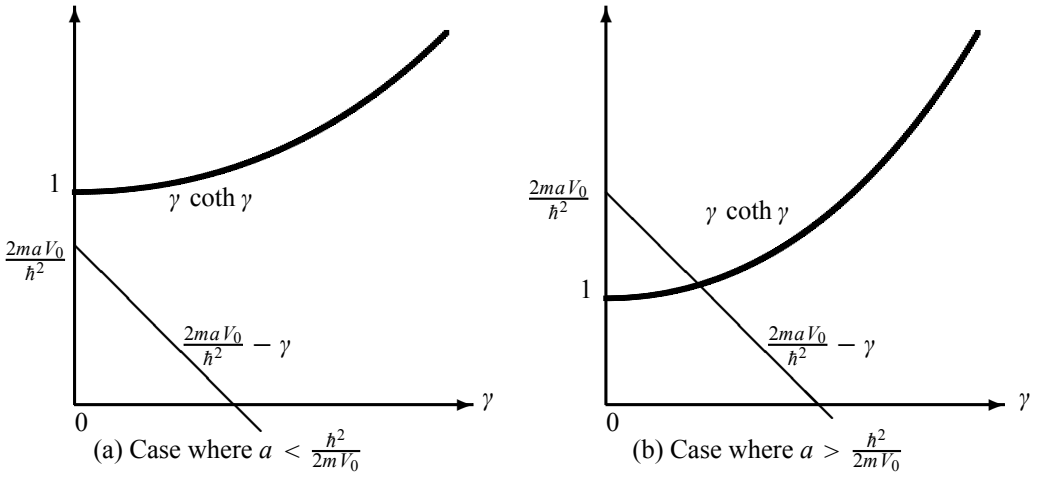


Figure 4.15 Graphical solutions of $h(\gamma) = u(\gamma)$, with $\gamma = ka$, $h(\gamma) = \gamma \coth \gamma$, and $u(\gamma) = 2mV_0a/\hbar^2 - \gamma$. If $a < 2mV_0/\hbar^2$ there is no bound state. If $a > 2mV_0/\hbar^2$ there is one bound state.

Problem 4.7
A particle of mass m, besides being confined to move inside an infinite square well potential of size a with walls at $x = 0$ and $x = a$, is subject to a delta potential of strength V_0

$$V(x) = \begin{cases} V_0\delta(x - a/2), & 0 < x < a, \\ \infty, & \text{elsewhere,} \end{cases}$$

where $V_0 > 0$. Show how to calculate the energy levels of the system in terms of V_0 and a.

Solution
The Schrödinger equation

$$\frac{d^2\psi(x)}{dx^2} + \frac{2mV_0}{\hbar^2}\delta\left(x - \frac{a}{2}\right)\psi(x) + \frac{2mE}{\hbar^2}\psi(x) = 0 \tag{4.275}$$

can be written for $x \neq a/2$ as

$$\frac{d^2\psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0. \tag{4.276}$$

The solutions of this equation must vanish at $x = 0$ and $x = a$:

$$\psi(x) = \begin{cases} \psi_L(x) = A \sin kx, & 0 \leq x < a/2, \\ \psi_R(x) = B \sin k(x - a), & a/2 < x \leq a, \end{cases} \tag{4.277}$$

where $k = \sqrt{2m|E|}/\hbar$. The continuity of $\psi(x)$ at $x = a/2$, $\psi_L(a/2) = \psi_R(a/2)$, leads to $A \sin(a/2) = -B \sin(a/2)$; hence $B = -A$. The wave function is thus given by

$$\psi(x) = \begin{cases} \psi_L(x) = A \sin kx, & 0 \leq x < a/2, \\ \psi_R(x) = -A \sin k(x - a), & a/2 < x \leq a, \end{cases} \tag{4.278}$$

The energy eigenvalues can be found from the discontinuity condition of the first derivative of the wave function, which in turn can be obtained by integrating (4.275) from $a/2-\varepsilon$ to $a/2+\varepsilon$ and then letting $\varepsilon \to 0$:

$$\lim_{\varepsilon\to 0}\left(\left.\frac{d\psi_R(x)}{dx}\right|_{x=a/2+\varepsilon} - \left.\frac{d\psi_L(x)}{dx}\right|_{x=a/2-\varepsilon}\right)_{\varepsilon=0} + \frac{2mV_0}{\hbar^2}\psi\left(\frac{a}{2}\right) = 0. \tag{4.279}$$

Substituting (4.278) into (4.279) we obtain

$$-kA\cos\left[k\left(\frac{a}{2}-a\right)\right] - kA\cos\left(k\frac{a}{2}\right) + A\frac{2mV_0}{\hbar^2}\sin\left(k\frac{a}{2}\right) = 0 \tag{4.280}$$

or

$$\tan\left(k\frac{a}{2}\right) = \frac{\hbar^2 k}{mV_0} \quad\Longrightarrow\quad \tan\left(\sqrt{\frac{ma^2|E|}{2\hbar^2}}\right) = \sqrt{\frac{2\hbar^2|E|}{mV_0^2}}. \tag{4.281}$$

This is a transcendental equation for the energy; its solutions, which can be obtained numerically or graphically, yield the values of E.

Problem 4.8
Using the uncertainty principle, show that the lowest energy of an oscillator is $\hbar\omega/2$.

Solution
The motion of the particle is confined to the region $-a/2 \le x \le a/2$; that is, $\Delta x \simeq a$. Then as a result of the uncertainty principle, the lowest value of this particle's momentum is $\hbar/(2\Delta x) \simeq \hbar/(2a)$. The total energy as a function of a is

$$E(a) \simeq \frac{1}{2m}\left(\frac{\hbar}{2a}\right)^2 + \frac{1}{2}m\omega^2 a^2. \tag{4.282}$$

The minimization of E with respect to a,

$$0 = \left.\frac{dE}{da}\right|_{a=a_0} = -\frac{\hbar^2}{4ma_0^3} + m\omega^2 a_0, \tag{4.283}$$

gives $a_0 = \sqrt{\hbar/2m\omega}$ and hence $E(a_0) \simeq \hbar\omega/2$; this is equal to the exact value of the oscillator's zero-point energy.

Problem 4.9
Find the energy levels of a particle of mass m moving in a one-dimensional potential:

$$V(x) = \begin{cases} +\infty, & x \le 0, \\ \frac{1}{2}m\omega^2 x^2, & x > 0. \end{cases}$$

Solution
This is an asymmetric harmonic oscillator potential in which the particle moves only in the region $x > 0$. The only acceptable solutions are those for which the wave function vanishes at $x = 0$. These solutions must be those of an ordinary (symmetric) harmonic oscillator that have odd parity, since the wave functions corresponding to the symmetric harmonic oscillator are

either even (n even) or odd (n odd), and only the odd solutions vanish at the origin, $\psi_{2n+1}(0) = 0$ ($n = 0, 1, 2, 3, \ldots$). Therefore, the energy levels of this asymmetric potential must be given by those corresponding to the odd n energy levels of the symmetric potential, i.e.,

$$E_n = \left[(2n+1) + \frac{1}{2}\right]\hbar\omega = \left(2n + \frac{3}{2}\right)\hbar\omega \qquad (n = 0, 1, 2, 3, \ldots). \tag{4.284}$$

Problem 4.10
Consider the box potential

$$V(x) = \begin{cases} 0, & 0 < x < a, \\ \infty, & \text{elsewhere.} \end{cases}.$$

(a) Estimate the energies of the ground state as well as those of the first and the second excited states for (i) an electron enclosed in a box of size $a = 10^{-10}$ m (express your answer in electron volts; you may use these values: $\hbar c = 200\,\text{MeV fm}$, $m_e c^2 = 0.5\,\text{MeV}$); (ii) a 1 g metallic sphere which is moving in a box of size $a = 10\,\text{cm}$ (express your answer in joules).

(b) Discuss the importance of the quantum effects for both of these two systems.

(c) Use the uncertainty principle to estimate the velocities of the electron and the metallic sphere.

Solution
The energy of a particle of mass m in a box having perfectly rigid walls is given by

$$E_n = \frac{n^2 h^2}{8ma^2}, \qquad n = 1, 2, 3, \ldots, \tag{4.285}$$

where a is the size of the box.

(a) (i) For the electron in the box of size 10^{-10} m, we have

$$\begin{aligned} E_n &= \frac{\hbar^2 c^2}{m_e c^2 a^2}\frac{4\pi^2 n^2}{8} \equiv \frac{4 \times 10^4\,(\text{MeV fm})^2}{0.5\,\text{MeV} \times 10^{10}\,\text{fm}^2}\frac{\pi^2}{2}n^2 \\ &= 4\pi^2 n^2\,\text{eV} \simeq 39n^2\,\text{eV}. \end{aligned} \tag{4.286}$$

Hence $E_1 = 39\,\text{eV}$, $E_2 = 156\,\text{eV}$, and $E_3 = 351\,\text{eV}$.

(ii) For the sphere in the box of side 10 cm we have

$$E_n = \frac{(6.6 \times 10^{-34}\,\text{J s})^2}{10^{-3}\,\text{kg} \times 10^{-2}\,\text{m}^2}n^2 = 43.6 \times 10^{-63} n^2\,\text{J} \tag{4.287}$$

Hence $E_1 = 43.6 \times 10^{-63}$ J, $E_2 = 174.4 \times 10^{-63}$ J, and $E_3 = 392.4 \times 10^{-63}$ J.

(b) The differences between the energy levels are

$$(E_2 - E_1)_{electron} = 117\,\text{eV}, \qquad (E_3 - E_2)_{electron} = 195\,\text{eV}, \tag{4.288}$$

$$(E_2 - E_1)_{sphere} = 130.8 \times 10^{-63}\,\text{J}, \qquad (E_3 - E_2)_{sphere} = 218 \times 10^{-63}\,\text{J}. \tag{4.289}$$

These results show that:

- The spacings between the energy levels of the electron are quite large; the levels are far apart from each other. Thus, the quantum effects are important.

- The energy levels of the sphere are practically indistinguishable; the spacings between the levels are negligible. The energy spectrum therefore forms a continuum; hence the quantum effects are not noticeable for the sphere.

(c) According to the uncertainty principle, the speed is proportional to $v \sim \hbar/(ma)$. For the electron, the typical distances are atomic, $a \simeq 10^{-10}$ m; hence

$$v \sim \frac{\hbar c}{mc^2 a} c \sim \frac{200\,\text{MeV fm}}{0.5\,\text{MeV} \times 10^5\,\text{fm}} c \simeq 4 \times 10^{-3} c = 1.2 \times 10^6 \text{m s}^{-1}, \tag{4.290}$$

where c is the speed of light. The electron therefore moves quite fast; this is expected since we have confined the electron to move within a small region.

For the sphere, the typical distances are in the range of 1 cm:

$$v \sim \frac{\hbar}{ma} \sim \frac{6.6 \times 10^{-34}\,\text{J s}}{10^{-3}\,\text{kg} \times 10^{-2}\,\text{m}} \simeq 6.6 \times 10^{-29} \text{m s}^{-1} \tag{4.291}$$

At this speed the sphere is practically at rest.

Problem 4.11

(a) Verify that the matrices representing the operators $\hat{X}$ and $\hat{P}$ in the N-space for a harmonic oscillator obey the correct commutation relation $[\hat{X},\ \hat{P}] = i\hbar$.

(b) Show that the energy levels of the harmonic oscillator can be obtained by inserting the matrices of $\hat{X}$ and $\hat{P}$ into the Hamiltonian $\hat{H} = \hat{P}^2/(2m) + \frac{1}{2}m\omega^2\hat{X}^2$.

Solution

(a) Using the matrices of $\hat{X}$ and $\hat{P}$ in (4.181) and (4.182), we obtain

$$\hat{X}\hat{P} = i\frac{\hbar}{2}\begin{pmatrix} 1 & 0 & -\sqrt{2} & \cdots \\ 0 & 1 & 0 & \cdots \\ \sqrt{2} & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \qquad \hat{P}\hat{X} = i\frac{\hbar}{2}\begin{pmatrix} -1 & 0 & -\sqrt{2} & \cdots \\ 0 & -1 & 0 & \cdots \\ \sqrt{2} & 0 & -1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}; \tag{4.292}$$

hence

$$\hat{X}\hat{P} - \hat{P}\hat{X} = i\hbar\begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{4.293}$$

or $[\hat{X},\ \hat{P}] = i\hbar I$, where I is the unit matrix.

(b) Again, using the matrices of $\hat{X}$ and $\hat{P}$ in (4.181) and (4.182), we can verify that

$$\hat{X}^2 = \frac{\hbar}{2m\omega}\begin{pmatrix} 1 & 0 & \sqrt{2} & \cdots \\ 0 & 3 & 0 & \cdots \\ \sqrt{2} & 0 & 5 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \qquad \hat{P}^2 = -\frac{m\hbar\omega}{2}\begin{pmatrix} -1 & 0 & \sqrt{2} & \cdots \\ 0 & -3 & 0 & \cdots \\ \sqrt{2} & 0 & -5 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}; \tag{4.294}$$

hence

$$\frac{\hat{P}^2}{2m} + \frac{1}{2}m\omega^2\hat{X}^2 = \frac{\hbar\omega}{2}\begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 3 & 0 & \cdots \\ 0 & 0 & 5 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{4.295}$$

The form of this matrix is similar to the result we obtain from an analytical treatment, $E_n = \hbar\omega(2n+1)/2$, since

$$H_{n'n} = \langle n'|\hat{H} \mid n\rangle = \frac{\hbar\omega}{2}(2n+1)\delta_{n'n}. \tag{4.296}$$

Problem 4.12
Calculate the probability of finding a particle in the classically forbidden region of a harmonic oscillator for the states $n = 0, 1, 2, 3, 4$. Are these results compatible with their classical counterparts?

Solution
The classical turning points are defined by $E_n = V(x_n)$ or by $\hbar\omega(n+\frac{1}{2}) = \frac{1}{2}m\omega^2 x_n^2$; that is, $x_n = \pm\sqrt{\hbar/(m\omega)}\sqrt{2n+1}$. Thus, the probability of finding a particle in the classically forbidden region for a state $\psi_n(x)$ is

$$P_n = \int_{-\infty}^{-|x_n|} |\psi_n(x)|^2\,dx + \int_{|x_n|}^{+\infty} |\psi_n(x)|^2\,dx = 2\int_{|x_n|}^{+\infty} |\psi_n(x)|^2\,dx, \tag{4.297}$$

where $\psi_n(x)$ is given in (4.172), $\psi_n(x) = 1/\sqrt{\sqrt{\pi}2^n n! x_0}e^{-x^2/2x_0^2}H_n(x/x_0)$, where x_0 is given by $x_0 = \sqrt{\hbar/(m\omega)}$. Using the change of variable $y = x/x_0$, we can rewrite P_n as

$$P_n = \frac{2}{\sqrt{\pi}2^n n!}\int_{\sqrt{2n+1}}^{+\infty} e^{-y^2}H_n^2(y)\,dy, \tag{4.298}$$

where the Hermite polynomials $H_n(y)$ are listed in (4.120). The integral in (4.298) can be evaluated only numerically. Using the numerical values

$$\int_1^\infty e^{-y^2}dy = 0.1394, \qquad \int_{\sqrt{3}}^\infty y^2 e^{-y^2}dy = 0.0495, \tag{4.299}$$

$$\int_{\sqrt{5}}^\infty \left(4y^2-2\right)^2 e^{-y^2}dy = 0.6740, \qquad \int_{\sqrt{7}}^\infty \left(8y^3-12y\right)^2 e^{-y^2}dy = 3.6363, \tag{4.300}$$

$$\int_{\sqrt{9}}^\infty \left(16y^4-48y^2+12\right)^2 e^{-y^2}dx = 26.86, \tag{4.301}$$

we obtain

$$P_0 = 0.1573, \qquad P_1 = 0.1116, \qquad P_2 = 0.095\,069, \tag{4.302}$$

$$P_3 = 0.085\,48, \qquad P_4 = 0.078\,93. \tag{4.303}$$

This shows that the probability decreases as n increases, so it would be very small for very large values of n. It is therefore unlikely to find the particle in the classically forbidden region when the particle is in a very highly excited state. This is what we expect, since the classical approximation is recovered in the limit of high values of n.

Problem 4.13
Consider a particle of mass m moving in the following potential

$$V(x) = \begin{cases} \infty, & x \leq 0, \\ -V_0, & 0 < x < a, \\ 0, & x \geq a, \end{cases}$$

where $V_0 > 0$.

(a) Find the wave function.

(b) Show how to obtain the energy eigenvalues from a graph.

(c) Calculate the minimum value of V_0 (in terms of m, a, and $\hbar$) so that the particle will have one bound state; then calculate it for two bound states. From these two results, try to obtain the lowest value of V_0 so that the system has n bound states.

Solution

(a) As shown in Figure 4.16, the wave function in the region $x < 0$ is zero, $\psi(x) = 0$. In the region $x > 0$ the Schrödinger equation for the bound state solutions, $-V_0 < E < 0$, is given by

$$\left(\frac{d^2}{dx^2} + k_1^2\right)\psi_1(x) = 0 \qquad (0 < x < a), \tag{4.304}$$

$$\left(\frac{d^2}{dx^2} - k_2^2\right)\psi_2(x) = 0 \qquad (x > a), \tag{4.305}$$

where $k_1^2 = 2m(V_0 + E)/\hbar^2$ and $k_2^2 = -2mE/\hbar^2$. On one hand, the solution of (4.304) is oscillatory, $\psi_1(x) = A \sin k_1 x + B \cos k_1 x$, but since $\psi_1(0) = 0$ we must have $B = 0$. On the other hand, eliminating the physically unacceptable solutions which grow exponentially for large values of x, the solution of (4.305) is $\psi_2(x) = Ce^{-k_2 x}$. Thus, the wave function is given by

$$\psi(x) = \begin{cases} 0, & x < 0, \\ \psi_1(x) = A \sin k_1 x, & 0 < x < 0, \\ \psi_2(x) = Ce^{-k_2 x}, & x > a. \end{cases} \tag{4.306}$$

(b) To determine the eigenvalues, we need to use the boundary conditions at $x = a$. The condition $\psi_1(a) = \psi_2(a)$ yields

$$A \sin k_1 a = Ce^{-k_2 a}, \tag{4.307}$$

while the continuity of the first derivative, $\psi_1'(a) = \psi_2\prime(a)$, leads to

$$Ak_1 \cos k_1 a = -Ck_2 e^{-k_2 a}. \tag{4.308}$$

Dividing (4.308) by (4.307) we obtain

$$k_1 a \cot k_1 a = -k_2 a. \tag{4.309}$$

Since $k_1^2 = 2m(V_0 + E)/\hbar^2$ and $k_2^2 = -2mE/\hbar^2$, we have

$$(k_1 a)^2 + (k_2 a)^2 = \gamma^2, \tag{4.310}$$

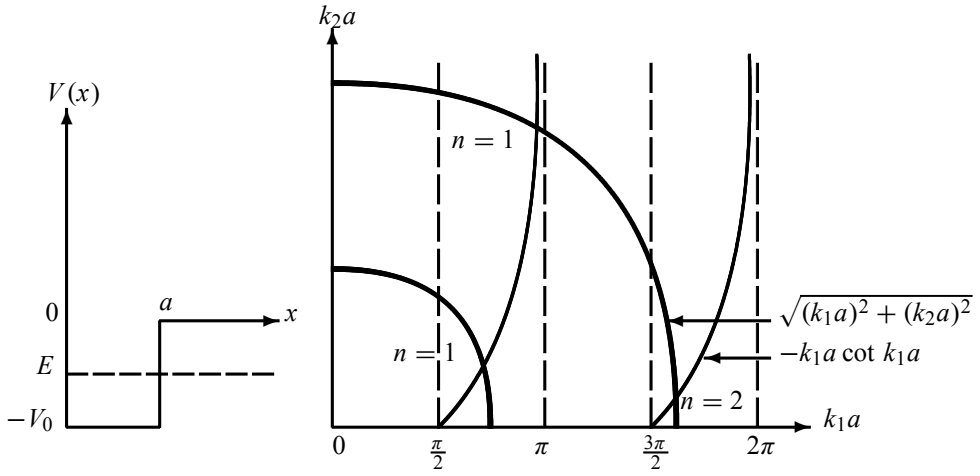


Figure 4.16 Potential $V(x)$ (left curve); the energy levels of $V(x)$ are given graphically by the intersection of the circular curve $\sqrt{(k_1a)^2 + (k_2a)^2}$ with $-k_1a \cot k_1a$ (right curve).

where $\gamma = \sqrt{2mV_0}a/\hbar$.

The transcendental equations (4.309) and (4.310) can be solved graphically. As shown in Figure 4.16, the energy levels are given by the intersection of the circular curve $(k_1a)^2 + (k_2a)^2 = \gamma^2$ with $k_1a \cot k_1a = -k_2a$.

(c) If $\pi/2 < \gamma < 3\pi/2$ there will be only one bound state, the ground state $n = 1$, for there is only one crossing between the curves $(k_1a)^2 + (k_2a)^2 = \gamma^2$ and $k_1a \cot k_1a = -k_2a$. The lowest value of V_0 that yields a single bound state is given by the relation $\gamma = \pi/2$, which leads to $2ma^2V_0/\hbar^2 = \pi^2/4$ or to

$$V_0 = \frac{\pi^2\hbar^2}{8ma^2}. \tag{4.311}$$

Similarly, if $3\pi/2 < \gamma < 5\pi/2$ there will be two crossings between $(k_1a)^2 + (k_2a)^2 = \gamma^2$ and $k_1a \cot k_1a = -k_2a$. Thus, there will be two bound states: the ground state, $n = 1$, and the first excited state, $n = 2$. The lowest value of V_0 that yields two bound states corresponds to $2ma^2V_0/\hbar^2 = 9\pi^2/4$ or to

$$V_0 = \frac{9\pi^2\hbar^2}{8ma^2}. \tag{4.312}$$

We may thus infer the following general result. If $n\pi - \pi/2 < \gamma < n\pi + \pi/2$, there will be n crossings and hence n bound states:

$$n\pi - \frac{\pi}{2} < \frac{\sqrt{2mV_0}}{\hbar}a < n\pi + \frac{\pi}{2} \quad \Longrightarrow \quad \text{there are } n \text{ bound states.} \tag{4.313}$$

The lowest value of V_0 giving n bound states is

$$V_0 = \frac{\pi^2\hbar^2}{8ma^2}(2n-1)^2. \tag{4.314}$$

Problem 4.14

(a) Assuming the potential seen by a neutron in a nucleus to be schematically represented by a one-dimensional, infinite rigid walls potential of length 10 fm, estimate the minimum kinetic energy of the neutron.

(b) Estimate the minimum kinetic energy of an electron bound within the nucleus described in (a). Can an electron be confined in a nucleus? Explain.

Solution

The energy of a particle of mass m in a one-dimensional box potential having perfectly rigid walls is given by

$$E_n = \frac{\pi^2\hbar^2}{2ma^2}n^2, \qquad n = 1, 2, 3, \ldots, \tag{4.315}$$

where a is the size of the box.

(a) Assuming the neutron to be nonrelativistic (i.e., its energy $E \ll m_nc^2$), the lowest energy the neutron can have in a box of size $a = 10$ fm is

$$E_{min} = \frac{\pi^2\hbar^2}{2m_na^2} = \frac{\pi^2(\hbar^2c^2)}{2(m_nc^2)a^2} \simeq 2.04\,\text{MeV}, \tag{4.316}$$

where we have used the fact that the rest mass energy of a neutron is $m_nc^2 \simeq 939.57$ MeV and $\hbar c \simeq 197.3$ MeV fm. Indeed, we see that $E_{min} \ll m_nc^2$.

(b) The minimum energy of a (nonrelativistic) electron moving in a box of size $a = 10$ fm is given by

$$E_{min} = \frac{\pi^2\hbar^2}{2m_ea^2} = \frac{\pi^2(\hbar^2c^2)}{2(m_ec^2)a^2} \simeq 3755.45\,\text{MeV}. \tag{4.317}$$

The rest mass energy of an electron is $m_ec^2 \simeq 0.511$ MeV, so this electron is ultra-relativistic since $E_{min} \gg m_ec^2$. It implies that an electron with this energy cannot be confined within such a nucleus.

Problem 4.15

(a) Calculate the expectation value of the operator $\hat{X}^4$ in the N-representation with respect to the state $|\,n\rangle$ (i.e., $\langle n \mid \hat{X}^4 \mid n\rangle$).

(b) Use the result of (a) to calculate the energy E_n for a particle whose Hamiltonian is $\hat{H} = \hat{P}^2/(2m) + \frac{1}{2}m\omega^2\hat{X}^2 - \lambda\hat{X}^4$.

Solution

(a) Since $\sum_{m=0}^{\infty} |m\rangle\langle m| = 1$ we can write the expectation value of $\hat{X}^4$ as

$$\langle n \mid \hat{X}^4 \mid n\rangle = \sum_{m=0}^{\infty}\langle n \mid \hat{X}^2|m\rangle\langle m|\hat{X}^2 \mid n\rangle = \sum_{m=0}^{\infty}\left|\langle m|\hat{X}^2 \mid n\rangle\right|^2. \tag{4.318}$$

Now since

$$\hat{X}^2 = \frac{\hbar}{2m\omega}\left(\hat{a}^2 + \hat{a}^{\dagger 2} + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}\right) = \frac{\hbar}{2m\omega}\left(\hat{a}^2 + \hat{a}^{\dagger 2} + 2\hat{a}^\dagger\hat{a} + 1\right), \tag{4.319}$$

the only terms $\langle m|\hat{X}^2 \mid n\rangle$ that survive are

$$\langle n \mid \hat{X}^2 \mid n\rangle = \frac{\hbar}{2m\omega}\langle n \mid 2\hat{a}^\dagger\hat{a} + 1 \mid n\rangle = \frac{\hbar}{2m\omega}(2n+1), \tag{4.320}$$

$$\langle n-2 \mid \hat{X}^2 \mid n\rangle = \frac{\hbar}{2m\omega}\langle n-2 \mid \hat{a}^2 \mid n\rangle = \frac{\hbar}{2m\omega}\sqrt{n(n-1)}, \tag{4.321}$$

$$\langle n+2 \mid \hat{X}^2 \mid n\rangle = \frac{\hbar}{2m\omega}\langle n+2 \mid \hat{a}^{\dagger 2} \mid n\rangle = \frac{\hbar}{2m\omega}\sqrt{(n+1)(n+2)}. \tag{4.322}$$

Thus

$$\begin{aligned}\langle n \mid \hat{X}^4 \mid n\rangle &= \left|\langle n \mid \hat{X}^2 \mid n\rangle\right|^2 + \left|\langle n-2 \mid \hat{X}^2 \mid n\rangle\right|^2 + \left|\langle n+2 \mid \hat{X}^2 \mid n\rangle\right|^2 \\ &= \frac{\hbar^2}{4m^2\omega^2}\left[(2n+1)^2 + n(n-1) + (n+1)(n+2)\right] \\ &= \frac{\hbar^2}{4m^2\omega^2}\left(6n^2+6n+3\right).\end{aligned} \tag{4.323}$$

(b) Using (4.323), and since the Hamiltonian can be expressed in terms of the harmonic oscillator, $\hat{H} = \hat{H}_{HO} - \lambda\hat{X}^4$, we immediately obtain the particle energy:

$$E_n = \langle n \mid \hat{H}_{HO} \mid n\rangle - \lambda\langle n \mid \hat{X}^4 \mid n\rangle = \hbar\omega\left(n+\frac{1}{2}\right) - \frac{\lambda\hbar^2}{4m^2\omega^2}\left(6n^2+6n+3\right). \tag{4.324}$$

Problem 4.16
Find the energy levels and the wave functions of two harmonic oscillators of masses m_1 and m_2, having identical frequencies ω, and coupled by the interaction $\frac{1}{2}k(\hat{X}_1 - \hat{X}_2)^2$.

Solution
This problem reduces to finding the eigenvalues for the Hamiltonian

$$\begin{aligned}\hat{H} &= \hat{H}_1 + \hat{H}_2 + \frac{1}{2}K(\hat{X}_1 - \hat{X}_2)^2 \\ &= \frac{1}{2m_1}\hat{P}_1^2 + \frac{1}{2}m_1\omega^2\hat{X}_1^2 + \frac{1}{2m_2}\hat{P}_2^2 + \frac{1}{2}m_2\omega^2\hat{X}_2^2 + \frac{1}{2}K(\hat{X}_1 - \hat{X}_2)^2.\end{aligned} \tag{4.325}$$

This is a two-particle problem. As in classical mechanics, it is more convenient to describe the dynamics of a two-particle system in terms of the center of mass (CM) and relative motions. For this, let us introduce the following operators:

$$\hat{P} = \hat{p}_1 + \hat{p}_2, \qquad \hat{X} = \frac{m_1\hat{x}_1 + m_2\hat{x}_2}{M}, \tag{4.326}$$

$$\hat{p} = \frac{m_2\hat{p}_1 - m_1\hat{p}_2}{M}, \qquad \hat{x} = \hat{x}_1 - \hat{x}_2, \tag{4.327}$$

where $M = m_1 + m_2$ and $\mu = m_1m_2/(m_1+m_2)$ is the reduced mass; $\hat{P}$ and $\hat{X}$ pertain to the CM; $\hat{p}$ and $\hat{x}$ pertain to the relative motion. These relations lead to

$$\hat{p}_1 = \frac{m_1}{M}\hat{P} + \hat{p}, \qquad \hat{p}_2 = \frac{m_2}{M}\hat{P} - \hat{p}, \tag{4.328}$$

$$\hat{x}_1 = \frac{m_2}{M}\hat{x} + \hat{X}, \qquad \hat{x}_2 = -\frac{m_1}{M}\hat{x} + \hat{X}. \tag{4.329}$$

Note that the sets (X, P) and (x, p) are conjugate variables separately: $[\hat{X}, \hat{P}] = i\hbar$, $[\hat{x}, \hat{p}] = i\hbar$, $[\hat{X}, \hat{p}] = [\hat{x}, \hat{P}] = 0$. Taking $\hat{p}_1$, $\hat{p}_2$, $\hat{x}_1$, and $\hat{x}_2$ of (4.328) and (4.329) and inserting them into (4.325), we obtain

$$\begin{aligned}\hat{H} &= \frac{1}{2m_1}\left(\frac{m_1}{M}\hat{P} + \hat{p}\right)^2 + \frac{1}{2}m_1\omega^2\left(\frac{m_2}{M}\hat{x} + \hat{X}\right)^2 \\ &\quad + \frac{1}{2m_2}\left(\frac{m_2}{M}\hat{P} - \hat{p}\right)^2 + \frac{1}{2}m_2\omega^2\left(-\frac{m_1}{M}\hat{x} + \hat{X}\right)^2 + \frac{1}{2}K\hat{x}^2 \\ &= \hat{H}_{CM} + \hat{H}_{rel}, \end{aligned} \tag{4.330}$$

where

$$\hat{H}_{CM} = \frac{1}{2M}\hat{P}^2 + \frac{1}{2}M\omega^2\hat{X}^2, \qquad \hat{H}_{rel} = \frac{1}{2\mu}\hat{p}^2 + \frac{1}{2}\mu\Omega^2\hat{x}^2, \tag{4.331}$$

with $\Omega^2 = \omega^2 + k/\mu$. We have thus reduced the Hamiltonian of these two coupled harmonic oscillators to the sum of two independent harmonic oscillators, one with frequency ω and mass M and the other of mass μ and frequency $\Omega = \sqrt{\omega^2 + k/\mu}$. That is, by introducing the CM and relative motion variables, we have managed to eliminate the coupled term from the Hamiltonian.

The energy levels of this two-oscillator system can be inferred at once from the suggestive Hamiltonians of (4.331):

$$E_{n_1 n_2} = \hbar\omega\left(n_1 + \frac{1}{2}\right) + \hbar\Omega\left(n_2 + \frac{1}{2}\right). \tag{4.332}$$

The states of this two-particle system are given by the product of the two states $|N\rangle = |n_1\rangle|n_2\rangle$; hence the total wave function, $\psi_n(X, x)$, is equal to the product of the center of mass wave function, $\psi_{n_1}(X)$, and the wave function of the relative motion, $\psi_{n_2}(x)$: $\psi_n(X, x) = \psi_{n_1}(X)\psi_{n_2}(x)$. Note that both of these wave functions are harmonic oscillator functions whose forms can be found in (4.172):

$$\psi_n(X, x) = \frac{1}{\sqrt{\pi}\sqrt{2^{n_1}2^{n_2}n_1!n_2!x_{0_1}x_{0_2}}} e^{-X^2/2x_{0_1}^2} e^{-x^2/2x_{0_2}^2} H_{n_1}\left(\frac{X}{x_{0_1}}\right) H_{n_2}\left(\frac{x}{x_{0_2}}\right), \tag{4.333}$$

where $n = (n_1,\ n_2)$, $x_{0_1} = \sqrt{\hbar/(M\omega)}$, and $x_{0_2} = \sqrt{\hbar/(\mu\Omega)}$.

Problem 4.17
Consider a particle of mass m and charge q moving under the influence of a one-dimensional harmonic oscillator potential. Assume it is placed in a constant electric field $\mathcal{E}$. The Hamiltonian of this particle is therefore given by $\hat{H} = \hat{P}^2/(2m) + \frac{1}{2}m\omega^2\hat{X}^2 - q\mathcal{E}\hat{X}$. Derive the energy expression and the wave function of the nth excited state.

Solution
To find the eigenenergies of the Hamiltonian

$$\hat{H} = \frac{1}{2m}\hat{P}^2 + \frac{1}{2}m\omega^2\hat{X}^2 - q\mathcal{E}\hat{X}, \tag{4.334}$$

it is convenient to use the change of variable $y = \hat{X} - q\mathcal{E}/(m\omega^2)$. Thus the Hamiltonian becomes

$$\hat{H} = \frac{1}{2m}\hat{P}^2 + \frac{1}{2}m\omega^2\hat{y}^2 - \frac{q^2\mathcal{E}^2}{2m\omega^2}. \tag{4.335}$$

Since the term $q^2\mathcal{E}^2/(2m\omega^2)$ is a mere constant and $\hat{P}^2/(2m) + \frac{1}{2}m\omega^2\hat{y}^2 = \hat{H}_{HO}$ has the structure of a harmonic oscillator Hamiltonian, we can easily infer the energy levels:

$$E_n = \langle n \mid \hat{H} \mid n \rangle = \hbar\omega\left(n + \frac{1}{2}\right) - \frac{q^2\mathcal{E}^2}{2m\omega^2}. \tag{4.336}$$

The wave function is given by $\psi_n(y) = \psi_n(x - q\mathcal{E}/(m\omega^2))$, where $\psi_n(y)$ is given in (4.172):

$$\psi_n(y) = \frac{1}{\sqrt{\sqrt{\pi}2^n n! x_0}} e^{-y^2/2x_0^2} H_n\left(\frac{y}{x_0}\right). \tag{4.337}$$

Problem 4.18
Consider a particle of mass m that is bouncing vertically and elastically on a smooth reflecting floor in the Earth's gravitational field

$$V(z) = \begin{cases} mgz, & z > 0, \\ +\infty, & z \leq 0, \end{cases},$$

where g is a constant (the acceleration due to gravity). Find the energy levels and wave function of this particle.

Solution
We need to solve the Schrödinger equation with the boundary conditions $\psi(0) = 0$ and $\psi(+\infty) = 0$:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(z)}{dz^2} + mgz\psi(z) = E\psi(z) \implies \frac{d^2\psi(z)}{dz^2} - \frac{2m}{\hbar^2}(mgz - E)\psi(z) = 0. \tag{4.338}$$

With the change of variable $x = (\hbar^2/(2m^2g))^{2/3}(2m/\hbar^2)(mgz - E)$, we can reduce this equation to

$$\frac{d^2\phi(x)}{dx^2} - x\phi(x) = 0. \tag{4.339}$$

This is a standard differential equation; its solution (which vanishes at $x \to= +\infty$, i.e., $\phi(+\infty) = 0$) is given by

$$\phi(x) = B\mathrm{Ai}(x) \qquad \text{where} \qquad \mathrm{Ai}(x) = \frac{1}{\pi}\int_0^\infty \cos\left(\frac{1}{3}t^3 + xt\right)dt, \tag{4.340}$$

where $\mathrm{Ai}(x)$ is called the *Airy function*.

When $z = 0$ we have $x = -(2/(mg^2\hbar^2))^{1/3}E$. The boundary condition $\psi(0) = 0$ yields $\phi[-(2/(mg^2\hbar^2))^{1/3}E] = 0$ or $\mathrm{Ai}[-(2/(mg^2\hbar^2))^{1/3}E] = 0$. The Airy function has zeros only at certain values of R_n: $\mathrm{Ai}(R_n) = 0$ with $n = 0, 1, 2, 3, \ldots$. The roots R_n of the Airy function can be found in standard tables. For instance, the first few roots are $R_0 = -2.338$, $R_1 = -4.088$, $R_2 = -5.521$, $R_3 = -6.787$.

The boundary condition $\psi(0) = 0$ therefore gives a *discrete* set of energy levels which can be expressed in terms of the roots of the Airy function:

$$\mathrm{Ai}\left[-\left(\frac{2}{mg^2\hbar^2}\right)^{1/3}E\right] = 0 \quad \implies \quad -\left(\frac{2}{mg^2\hbar^2}\right)^{1/3}E_n = R_n; \tag{4.341}$$

hence

$$E_n = -\left(\frac{1}{2}mg^2\hbar^2\right)^{1/3} R_n, \qquad \psi_n(z) = B_n \mathrm{Ai}\left[-\left(\frac{2m^2g^2}{\hbar^2}\right)^{1/3} z - R_n\right]. \tag{4.342}$$

The first few energy levels are

$$E_0 = 2.338\left(\frac{1}{2}mg^2\hbar^2\right)^{1/3}, \qquad E_1 = 4.088\left(\frac{1}{2}mg^2\hbar^2\right)^{1/3}, \tag{4.343}$$

$$E_2 = 5.521\left(\frac{1}{2}mg^2\hbar^2\right)^{1/3}. \qquad E_3 = 6.787\left(\frac{1}{2}mg^2\hbar^2\right)^{1/3}. \tag{4.344}$$

4.11 Exercises

Exercise 4.1
A particle of mass m is subjected to a potential

$$V(x) = \begin{cases} 0, & |x| < a/2, \\ \infty, & |x| > a/2. \end{cases}$$

(a) Find the ground, first, and second excited state wave functions.
(b) Find expressions for E_1, E_2, and E_3.
(c) Plot the probability densities $P_2(x,t)$ and $P_3(x,t)$.
(d) Find $\langle X\rangle_2$, $\langle X\rangle_3$, $\langle P\rangle_2$, and $\langle P\rangle_3$.
(e) Evaluate $\Delta x\,\Delta p$ for the states $\psi_2(x,t)$ and $\psi_3(x,t)$.

Exercise 4.2
Consider a system whose wave function at $t = 0$ is

$$\psi(x,0) = \frac{3}{\sqrt{30}}\phi_0(x) + \frac{4}{\sqrt{30}}\phi_1(x) + \frac{1}{\sqrt{6}}\phi_4(x),$$

where $\phi_n(x)$ is the wave function of the nth excited state of an infinite square well potential of width a and whose energy is $E_n = \pi^2\hbar^2n^2/(2ma^2)$.

(a) Find the average energy of this system.

(b) Find the state $\psi(x,t)$ at a later time t and the average value of the energy. Compare the result with the value obtained in (a).

Exercise 4.3
An electron with a kinetic energy of 10 eV at large negative values of x is moving from left to right along the x-axis. The potential energy is

$$V(x) = \begin{cases} 0 & (x \le 0), \\ 20\,\mathrm{eV} & (x > 0). \end{cases}$$

(a) Write the time-independent Schrödinger equation in the regions $x \le 0$ and $x > 0$.
(b) Describe the shapes for $\psi(x)$ for $x \le 0$ and $x > 0$.

(c) Calculate the electron wavelength (in meters) in $-20\,\text{m} < x < -10\,\text{m}$ and $x > 10\,\text{m}$.

(d) Write down the boundary conditions at $x = 0$.

(e) Calculate the ratio of the probabilities for finding the electron near $x = 10^{-10}\,\text{m}$ and $x = 0$.

Exercise 4.4

A particle is moving in the potential well

$$V(x) = \begin{cases} 0, & -a \le x \le -b, \\ V_0, & -b \le x \le b, \\ 0, & b \le x \le a, \\ +\infty & \text{elsewhere} \end{cases},$$

where V_0 is positive. In this problem consider $E < V_0$. Let $\psi_1(x)$ and $\psi_2(x)$ represent the two lowest energy solutions of the Schrödinger equation; call their energies E_1 and E_2, respectively.

(a) Calculate E_1 and E_2 in units of eV for the case where $mc^2 = 1\,\text{GeV}$, $a = 10^{-14}\,\text{m}$, and $b = 0.4 \times 10^{-14}\,\text{m}$; take $\hbar c \simeq 200\,\text{MeV fm}$.

(b) A particular solution of the Schrödinger equation can be constructed by superposing $\psi_1(x)e^{iE_1t/\hbar}$ and $\psi_2(x)e^{iE_2t/\hbar}$. Construct a wave packet ψ which at $t = 0$ is (almost) entirely to the left-hand side of the well and describe its motion in time; find the period of oscillations between the two terms of ψ.

Exercise 4.5

A particle moves in the potential

$$V(x) = \frac{\hbar^2}{2m}\left[\frac{4}{225}\sinh^2 x - \frac{2}{5}\cosh x\right].$$

(a) Sketch $V(x)$ and locate the position of the two minima.

(b) Show that $\psi(x) = (1+4\cosh x)\exp\left(-\frac{2}{15}\cosh x\right)$ is a solution of the time-independent Schrödinger equation for the particle. Find the corresponding energy level and indicate its position on the sketch of $V(x)$.

(c) Sketch $\psi(x)$ and show that it has the proper behavior at the classical turning points and in the classically forbidden regions.

Exercise 4.6

Show that for a particle of mass m which moves in a one-dimensional infinite potential well of length a, the uncertainties product $\Delta x_n \Delta p_n$ is given by $\Delta x_n \Delta p_n \simeq n\pi\hbar/\sqrt{12}$.

Exercise 4.7

A particle of mass m is moving in an infinite potential well

$$V(x) = \begin{cases} V_0, & 0 < x < a, \\ \infty, & \text{elsewhere.} \end{cases}$$

(a) Solve the Schrödinger equation and find the energy levels and the corresponding normalized wave functions.

(b) Calculate $\langle\hat{X}\rangle_5$, $\langle\hat{P}\rangle_5$, $\langle\hat{X}^2\rangle_5$, and $\langle\hat{P}^2\rangle_5$ for the fourth excited state and infer the value of $\Delta x\,\Delta p$.

Exercise 4.8
Consider the potential step

$$V(x) = \begin{cases} 6\,\text{eV}, & x < 0, \\ 0, & x > 0. \end{cases}$$

(a) An electron of energy 8 eV is moving from left to right in this potential. Calculate the probability that the electron will (i) continue moving along its initial direction after reaching the step and (ii) get reflected at the potential step.

(b) Now suppose the electron is moving from right to left with an energy 3 eV. (i) Estimate the order of magnitude of the distance the electron can penetrate the barrier. (ii) Repeat part (i) for a 70 kg person initially moving at $4\,\text{m}\,\text{s}^{-1}$ and running into a wall which can be represented by a potential step of height equal to four times this person's energy before reaching the step.

Exercise 4.9
Consider a system whose wave function at time $t = 0$ is given by

$$\psi(x,0) = \frac{5}{\sqrt{50}}\phi_0(x) + \frac{4}{\sqrt{50}}\phi_1(x) + \frac{3}{\sqrt{50}}\phi_2(x),$$

where $\phi_n(x)$ is the wave function of the nth excited state for a harmonic oscillator of energy $E_n = \hbar\omega(n + 1/2)$.

(a) Find the average energy of this system.

(b) Find the state $\psi(x,t)$ at a later time t and the average value of the energy; compare the result with the value obtained in (a).

(c)Find the expectation value of the operator $\hat{X}$ with respect to the state $\psi(x,t)$ (i.e., find $\langle\psi(x,t)|\hat{X}|\psi(x,t)\rangle$).

Exercise 4.10
Calculate $\langle n \mid \hat{X}^2 \mid m\rangle$ and $\langle m \mid \hat{X}^4 \mid n\rangle$ in the N-representation; $\mid n\rangle$ and $\mid m\rangle$ are harmonic oscillator states.

Exercise 4.11
Consider the dimensionless Hamiltonian $\hat{H} = \frac{1}{2}\hat{P}^2 + \frac{1}{2}\hat{X}^2$, with $\hat{P} = -id/dx$.

(a) Show that the wave functions $\psi_0(x) = e^{-x^2/2}/\sqrt{\sqrt{\pi}}$ and $\psi_1(x) = \sqrt{2/\sqrt{\pi}}xe^{-x^2/2}$ are eigenfunctions of $\hat{H}$ with eigenvalues $1/2$ and $3/2$, respectively.

(b) Find the values of the coefficients α and β such that

$$\psi_2(x) = \frac{1}{\sqrt{2\sqrt{\pi}}}\left(\alpha x^2 - 1\right)e^{-x^2/2} \quad \text{and} \quad \psi_3(x) = \frac{1}{\sqrt{6\sqrt{\pi}}}x\left(1 + \beta x^2\right)e^{-x^2/2}$$

are orthogonal to $\psi_0(x)$ and $\psi_1(x)$, respectively. Then show that $\psi_2(x)$ and $\psi_3(x)$ are eigenfunctions of $\hat{H}$ with eigenvalues $5/2$ and $7/2$, respectively.

Exercise 4.12
Consider the dimensionless Hamiltonian $\hat{H} = \frac{1}{2}\hat{P}^2 + \frac{1}{2}\hat{X}^2$ (with $\hat{P} = -id/dx$) whose wave function at time $t = 0$ is given by

$$\Psi(x,0) = \frac{1}{\sqrt{2}}\psi_0(x) + \frac{1}{\sqrt{8}}\psi_1(x) + \frac{1}{\sqrt{10}}\psi_2(x),$$

where $\psi_0(x) = \frac{1}{\sqrt{\sqrt{\pi}}} e^{-x^2/2}$, $\psi_1(x) = \sqrt{\frac{2}{\sqrt{\pi}}} x e^{-x^2/2}$, and $\psi_2(x) = \frac{1}{\sqrt{2\sqrt{\pi}}} \left(2x^2 - 1\right) e^{-x^2/2}$.

(a) Calculate $\Delta x_n \Delta p_n$ for $n = 0, 1$ where $\Delta x_n = \sqrt{\langle \psi_n | \hat{X}^2 | \psi_n \rangle - \langle \psi_n | \hat{X} | \psi_n \rangle^2}$.

(b) Calculate $\hat{a}^\dagger \psi_0(x)$, $\hat{a} \psi_0(x)$, $\hat{a}^\dagger \psi_1(x)$, $\hat{a} \psi_1(x)$, and $\hat{a} \psi_2(x)$, where the operators $\hat{a}^\dagger$ and $\hat{a}$ are defined by $\hat{a} = (\hat{X} + d/dx)/\sqrt{2}$ and $\hat{a}^\dagger = (\hat{X} - d/dx)/\sqrt{2}$.

Exercise 4.13
Consider a particle of mass m that is moving in a one-dimensional infinite potential well with walls at $x = 0$ and $x = a$ which is initially (i.e., at $t = 0$) in the state

$$\psi(x, 0) = \frac{1}{\sqrt{2}} \left[\phi_1(x) + \phi_3(x)\right],$$

where $\phi_1(x)$ and $\phi_3(x)$ are the ground and second excited states, respectively.

(a) What is the state vector $\psi(x, t)$ for $t > 0$ in the Schrödinger picture.

(b) Find the expectation values $\langle \hat{X} \rangle$, $\langle \hat{P} \rangle$, $\langle \hat{X}^2 \rangle$, and $\langle \hat{P}^2 \rangle$ with respect to $| \psi \rangle$.

(c) Evaluate $\Delta x \Delta p$ and verify that it satisfies the uncertainty principle.

Exercise 4.14
If the state of a particle moving in a one-dimensional harmonic oscillator is given by

$$| \psi \rangle = \frac{1}{\sqrt{17}} | 0 \rangle + \frac{3}{\sqrt{17}} | 1 \rangle - \frac{2}{\sqrt{17}} | 2 \rangle - \sqrt{\frac{3}{17}} | 3 \rangle,$$

where $| n \rangle$ represents the normalized nth energy eigenstate, find the expectation values of the number operator, $\hat{N}$, and of the Hamiltonian operator.

Exercise 4.15
Find the number of bound states and the corresponding energies for the finite square well potential when (a) $R = 7$ (i.e., $\sqrt{ma^2 V_0/(2\hbar^2)} = 7$) and (b) $R = 3\pi$.

Exercise 4.16
A ball of mass $m = 0.2$ kg bouncing on a table located at $z = 0$ is subject to the potential

$$V(z) = \begin{cases} V_0 & (z < 0), \\ mgz & (z > 0), \end{cases}$$

where $V_0 = 3$ J and g is the acceleration due to gravity.

(a) Describe the spectrum of possible energies (i.e., continuous, discrete, or nonexistent) as E increases from large negative values to large positive values.

(b) Estimate the order of magnitude for the lowest energy state.

(c) Describe the general shapes of the wave functions $\psi_0(z)$ and $\psi_1(z)$ corresponding to the lowest two energy states and sketch the corresponding probability densities.

Exercise 4.17
Consider a particle of mass m moving in a one-dimensional harmonic oscillator potential, with $\hat{X} = \sqrt{\hbar/(2m\omega)}(\hat{a} + \hat{a}^\dagger)$ and $\hat{P} = i\sqrt{m\hbar\omega/2}(\hat{a}^\dagger - \hat{a})$.

(a) Calculate the product of the uncertainties in position and momentum for the particle in the fifth excited state, i.e., $(\Delta X \Delta P)_5$.

(b) Compare the result of (a) with the uncertainty product when the particle is in its lowest energy state. Explain why the two uncertainty products are different.

Exercise 4.18
A particle of mass m in an infinite potential well of length a has the following initial wave function at $t = 0$:

$$\psi(x, 0) = \frac{2}{\sqrt{7a}} \sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{6}{7a}} \sin\left(\frac{2\pi x}{a}\right) + \frac{2}{\sqrt{7a}} \sin\left(\frac{3\pi x}{a}\right).$$

(a) If we measure energy, what values will we find and with what probabilities? Calculate the average energy.

(b) Find the wave function $\psi(x, t)$ at any later time t. Determine the probability of finding the particle at a time t in the state $\varphi(x, t) = 1/\sqrt{a} \sin(3\pi x/a) \exp(-i E_3 t/\hbar)$.

(c) Calculate the probability density $\rho(x, t)$ and the current density $\vec{J}(x, t)$. Verify that $\partial\rho/\partial t + \vec{\nabla} \cdot \vec{J}(x, t) = 0$.

Exercise 4.19
Consider a particle in an infinite square well whose wave function is given by

$$\psi(x) = \begin{cases} Ax(a^2 - x^2), & 0 < x < a, \\ 0, & \text{elsewhere,} \end{cases}$$

where A is a real constant.

(a) Find A so that $\psi(x)$ is normalized.

(b) Calculate the position and momentum uncertainties, Δx and Δp, and the product $\Delta x \, \Delta p$.

(c) Calculate the probability of finding $5^2\pi^2\hbar^2/(2ma^2)$ for a measurement of the energy.

Exercise 4.20
The relativistic expression for the energy of a free particle is $E^2 = m_0^2 \, c^4 + p^2 \, c^2$.

(a) Write down the corresponding relativistic Schrödinger equation, by quantizing this energy expression (i.e., replacing E and p with their corresponding operators). This equation is called the Klein–Gordon equation.

(b) Find the solutions corresponding to a free particle moving along the x-axis.

Exercise 4.21
(a) Write down the classical (gravitational) energy E_c of a particle of mass m at rest a height h_0 above the ground (take the zero potential energy to be located at the ground level).

(b) Use the uncertainty principle to estimate the ground state energy E_0 of the particle introduced in (a); note that the particle is subject to gravity. Compare E_0 to E_c.

(c) If $h_0 = 3\,\text{m}$ obtain the numerical values of E_c and the quantum mechanical correction $(E_0 - E_c)$ for a neutron and then for a particle of mass $m = 0.01\,\text{kg}$. Comment on the importance of the quantum correction in both cases.

Exercise 4.22
Find the energy levels and the wave functions of two noninteracting particles of masses m_1 and m_2 that are moving in a common infinite square well potential

$$V(x_i) = \begin{cases} 0, & 0 \le x_i \le a, \\ +\infty, & \text{elsewhere,} \end{cases}$$

where x_i is the position of the ith particle (i.e., x_i denotes $x = x_1$ or x_2).

Exercise 4.23
A particle of mass m is subject to a repulsive delta potential $V(x) = V_0\delta(x)$, where $V_0 > 0$ (V_0 has the dimensions of Energy×Distance). Find the reflection and transmission coefficients, R and T.

Exercise 4.24
A particle of mass m is scattered by a double-delta potential $V(x) = V_0\delta(x-a) + V_0\delta(x+a)$, where $V_0 > 0$.

(a) Find the transmission coefficient for the particle at an energy $E > 0$.

(b) When V_0 is very large (i.e., $V_0 \to \infty$), find the energies corresponding to the resonance case (i.e., $T = 1$) and compare them with the energies of an infinite square well potential having a width of $2a$.

Exercise 4.25
A particle of mass m is subject to an antisymmetric delta potential $V(x) = V_0\delta(x+a) - V_0\delta(x-a)$, where $V_0 > 0$.

(a) Show that there is always one and only one bound state, and find the expression that gives its energy.

(b) Find the transmission coefficient T.

Exercise 4.26
A particle of mass m is subject to a delta potential

$$V(x) = \begin{cases} \infty, & x \leq 0, \\ V_0\delta(x-a), & x > 0, \end{cases}$$

where $V_0 > 0$.

(a) Find the wave functions corresponding to the cases $0 < x < a$ and $x > a$.

(b) Find the transmission coefficient.

Exercise 4.27
A particle of mass m, besides being confined to move in an infinite square well potential of size $2a$ with walls at $x = -a$ and $x = a$, is subject to an attractive delta potential

$$V(x) = \begin{cases} V_0\delta(x), & -a < x < a, \\ \infty, & \text{elsewhere}, \end{cases}$$

where $V_0 > 0$.

(a) Find the particle's wave function corresponding to *even* solutions when $E > 0$.

(b) Find the energy levels corresponding to *even* solutions.

Exercise 4.28
A particle of mass m, besides being confined to move in an infinite square well potential of size $2a$ with walls at $x = -a$ and $x = a$, is subject to an attractive delta potential

$$V(x) = \begin{cases} V_0\delta(x), & -a < x < a, \\ \infty, & \text{elsewhere}, \end{cases}$$

where $V_0 > 0$.

(a) Find the particle's wave function corresponding to *odd* solutions when $E > 0$.

(b) Find the energy levels corresponding to *odd* solutions.

Exercise 4.29
Consider a particle of mass m that is moving under the influence of an attractive delta potential

$$V(x) = \begin{cases} -V_0\delta(x), & x > -a, \\ \infty, & x < -a, \end{cases}$$

where $V_0 > 0$. Discuss the existence of bound states in terms of V_0 and a.

Exercise 4.30
Consider a system of two identical harmonic oscillators (with an angular frequency ω).

(a) Find the energy levels when the oscillators are independent (non-interacting).

(b) Find the energy levels when the oscillators are coupled by an interaction $-\lambda\hat{X}_1\hat{X}_2$, where λ is a constant.

(c) Assuming that $\lambda \ll m\omega^2$ (weak coupling limit), find an approximate value to first order in $\lambda/m\omega^2$ for the energy expression derived in part (b).

Exercise 4.31
A particle is initially in its ground state in an infinite one-dimensional potential box with sides at $x = 0$ and $x = a$. If the wall of the box at $x = a$ is *suddenly* moved to $x = 3a$, calculate the probability of finding the particle in

(a) the ground state of the new box and

(b) the first excited state of the new box.

(c) Now, calculate the probability of finding the particle in the first excited state of the new box, assuming the particle was initially in the first excited state of the old box.

Exercise 4.32
A particle is initially in its ground state in a one-dimensional harmonic oscillator potential, $\hat{V}(x) = \frac{1}{2}k\hat{x}^2$. If the spring constant is *suddenly* doubled, calculate the probability of finding the particle in the ground state of the new potential.

Exercise 4.33
Consider an electron in an infinite potential well

$$V(x) = \begin{cases} 0, & 0 < x < a, \\ +\infty, & \text{elsewhere}, \end{cases}$$

where $a = 10^{-10}$ m.

(a) Calculate the energy levels of the three lowest states (the results should be expressed in eV) and the corresponding wavelengths of the electron.

(b) Calculate the frequency of the radiation that would cause the electron to jump from the ground to the third excited energy level.

(c) When the electron de-excites, what are the frequencies of the emitted photons?

(d) Specify the probability densities for all these three states and plot them.

Exercise 4.34
Consider an electron which is confined to move in an infinite square well of width $a = 10^{-10}m$.

(a) Find the exact energies of the 11 lowest states (express them in eV).

(b) Solve the Schrödinger equation *numerically* and find the energies of the 11 lowest states and compare them with the exact results obtained in (a). Plot the wave functions of the five lowest states.