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):

$$\psi(x) = \begin{cases} \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}, & x \le 0, \\ \psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}, & 0 < x < a, \\ \psi_3(x) = Ee^{ik_1x}, & x \ge a, \end{cases} \tag{4.36}$$

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:

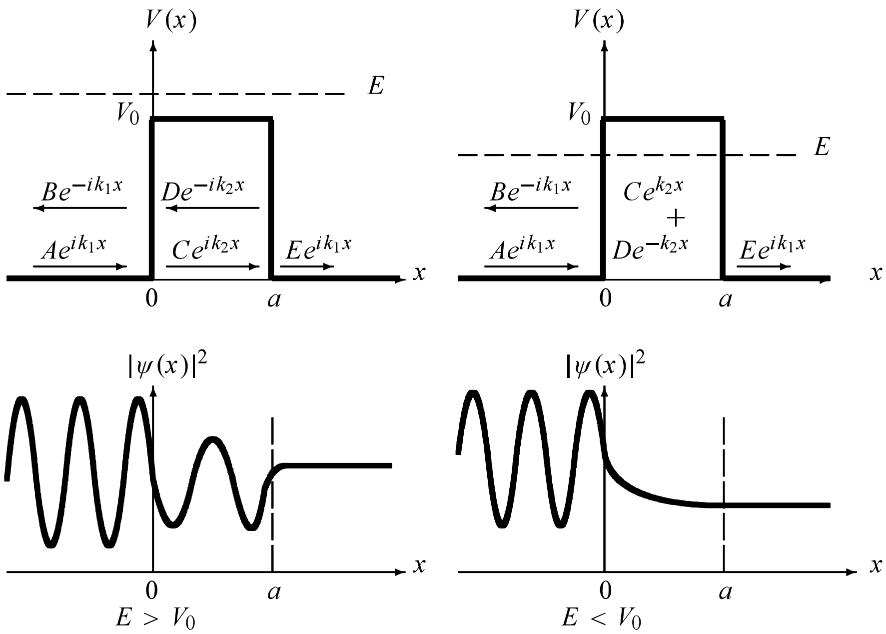

Figure 4.3 Potential barrier and propagation directions of the incident, reflected, and transmitted waves, plus their probability densities $|\psi(x)|^2$ when $E > V_0$ and $E < V_0$.

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

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

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

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

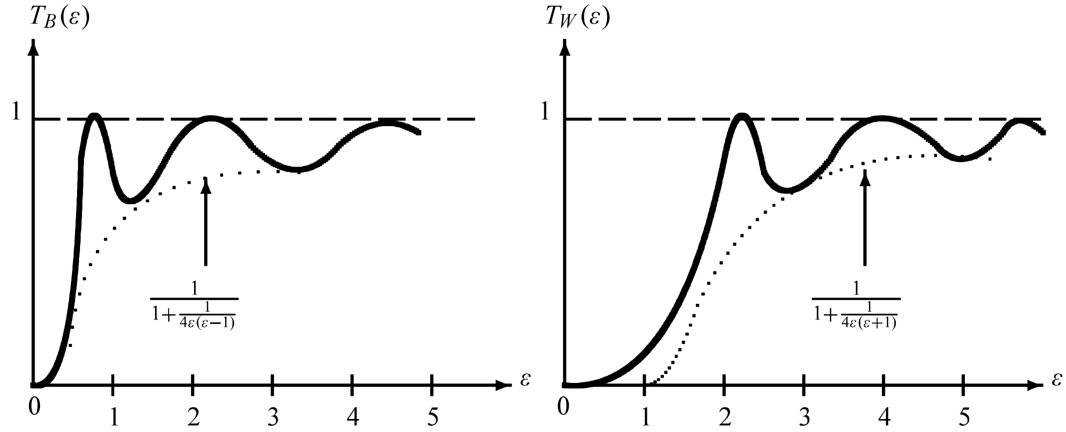

Figure 4.4 Transmission coefficients for a potential barrier, $T_B(\varepsilon) = \frac{4\varepsilon(\varepsilon-1)}{4\varepsilon(\varepsilon-1)+\sin^2(\lambda\sqrt{\varepsilon-1})}$, and for a potential well, $T_W(\varepsilon) = \frac{4\varepsilon(\varepsilon+1)}{4\varepsilon(\varepsilon+1)+\sin^2(\lambda\sqrt{\varepsilon+1})}$.

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

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

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

$$1 + \frac{B}{A} = \frac{E}{A}e^{ik_1 a}\left[\cosh(k_2 a) - i\frac{k_1}{k_2}\sinh(k_2 a)\right], \tag{4.55}$$

$$1 - \frac{B}{A} = \frac{E}{A}e^{ik_1 a}\left[\cosh(k_2 a) + i\frac{k_2}{k_1}\sinh(k_2 a)\right]. \tag{4.56}$$

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

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

$$\frac{E}{A} = 2e^{-ik_1 a}\left[2\cosh(k_2 a) + i\frac{k_2^2 - k_1^2}{k_1 k_2}\sinh(k_2 a)\right]^{-1}. \tag{4.58}$$

Thus, the coefficients R and T become

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

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

We can rewrite R in terms of T as

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

Since $\cosh^2(k_2 a) = 1 + \sinh^2(k_2 a)$ we can reduce (4.60) to

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

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:

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

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

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

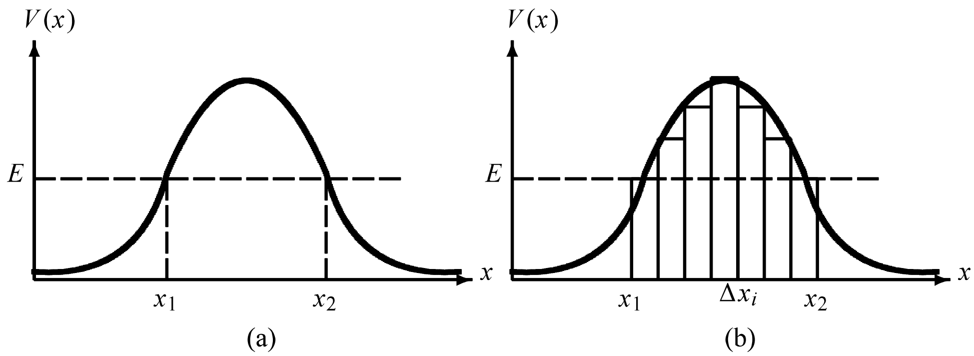

Figure 4.5 (a) Tunneling though a potential barrier. (b) Approximation of a smoothly varying potential $V(x)$ by square barriers.

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

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

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

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

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

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

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 $0 \leq x \leq a$, 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 $n \to \infty$,

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