PHYS1001B College Physics IB

Modern Physics III QUANTUM MECHANICS (Ch. 40)

Introduction

Quantum mechanics? Microscopic level

Particle-wave duality

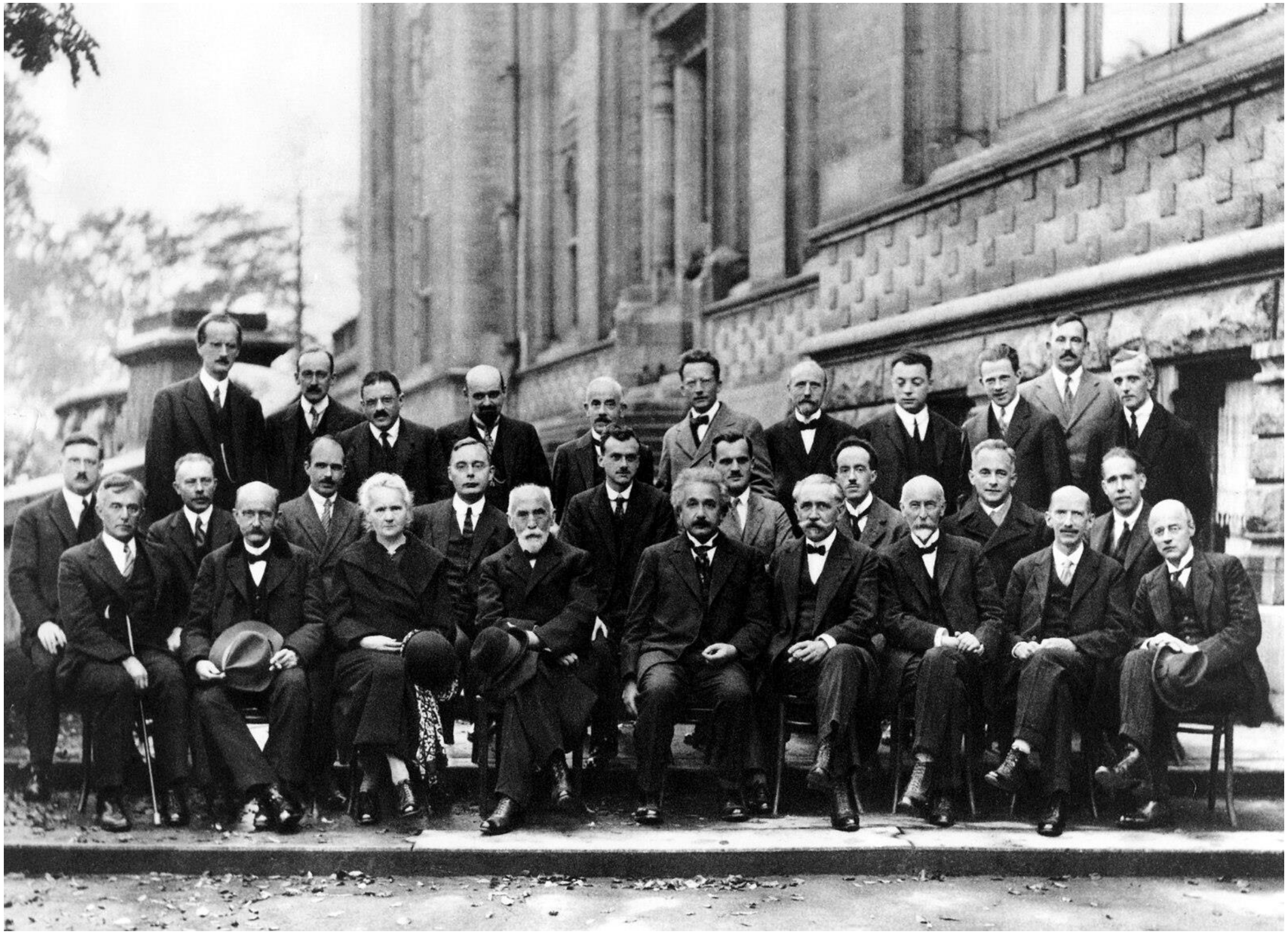
Uncertainty principle with Planck constant

Quantized energy with Planck constant

Introduction

40.4 In 1926, the German physicist Max Born (1882–1970) devised the interpretation that $|\Psi|^2$ is the probability distribution function for a particle that is described by the wave function Ψ. He also coined the term "quantum mechanics" (in the original German, *Quantenmechanik*). For his contributions, Born shared (with Walther Bothe) the 1954 Nobel Prize in physics.

Introduction



Solvay Conference: joint efforts of great scientists

Outline

- 40-1 Wave Functions and the One-Dimensional Schrodinger Equation
- 40-2 Particle in a Box
- 40-3 Potential Wells
- 40-4 Potential Barriers and Tunneling

40-1 Wave Functions and the One-Dimensional Schrodinger Equation

Wave equation

$$\frac{\partial^2 y(x,t)}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y(x,t)}{\partial t^2} \qquad \text{(wave equation for waves on a string)}$$

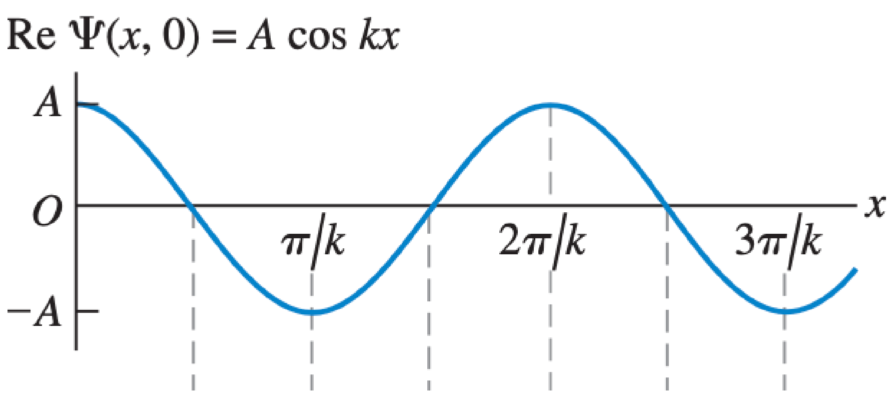
$$y(x,t) = A\cos(kx - \omega t) + B\sin(kx - \omega t) \qquad \text{(sinusoidal wave on a string)}$$

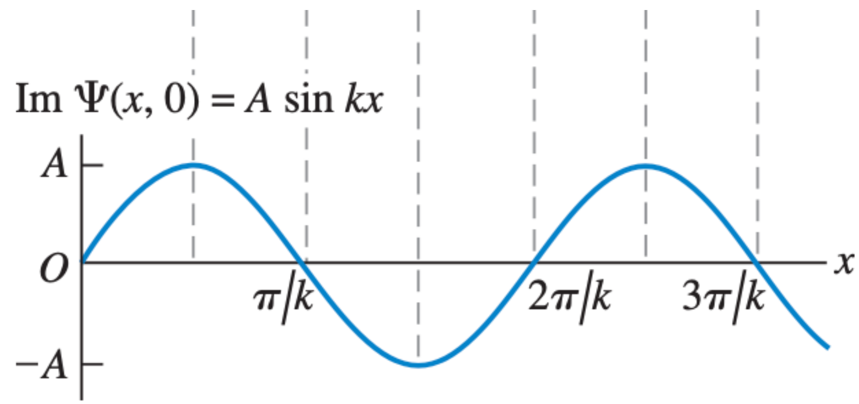
40-1 Wave Functions and the One-Dimensional Schrodinger Equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$ (one-dimensional Schrödinger equation for a free particle)

$$\Psi(x,t) = A[\cos(kx - \omega t) + i\sin(kx - \omega t)]$$ (sinusoidal wave function representing a free particle)

$$\Psi(x,t) = Ae^{i(kx-\omega t)} = Ae^{ikx}e^{-i\omega t}$$





Sample Problem

Example 40.1 A localized free-particle wave function

The wave function $\Psi(x, t) = Ae^{i(k_1x-\omega_1t)} + Ae^{i(k_2x-\omega_2t)}$ is a superposition of *two* free-particle wave functions of the form given by Eq. (40.18). Both k_1 and k_2 are positive. (a) Show that this wave function satisfies the Schrödinger equation for a free particle of mass m. (b) Find the probability distribution function for $\Psi(x, t)$.

Sample Problem

EXECUTE: (a) If we substitute $\Psi(x, t)$ into Eq. (40.15), the left-hand side of the equation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} = -\frac{\hbar^2}{2m}\frac{\partial^2(Ae^{i(k_1x-\omega_1t)} + Ae^{i(k_2x-\omega_2t)})}{\partial x^2}$$

$$= -\frac{\hbar^2}{2m}\left[(ik_1)^2Ae^{i(k_1x-\omega_1t)} + (ik_2)^2Ae^{i(k_2x-\omega_2t)}\right]$$

$$= \frac{\hbar^2k_1^{\,2}}{2m}Ae^{i(k_1x-\omega_1t)} + \frac{\hbar^2k_2^{\,2}}{2m}Ae^{i(k_2x-\omega_2t)}$$

The right-hand side is

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = i\hbar\frac{\partial(Ae^{i(k_1x-\omega_1t)} + Ae^{i(k_2x-\omega_2t)})}{\partial t}$$

$$= i\hbar\left[(-i\omega_1)Ae^{i(k_1x-\omega_1t)} + (-i\omega_2)Ae^{i(k_2x-\omega_2t)}\right]$$

$$= \hbar\omega_1Ae^{i(k_1x-\omega_1t)} + \hbar\omega_2Ae^{i(k_2x-\omega_2t)}$$

The two sides *are* equal, provided that $\hbar\omega_1 = \hbar^2k_1^{\,2}/2m$ and $\hbar\omega_2 = \hbar^2k_2^{\,2}/2m$. These are just the relationships that we noted

Sample Problem

(b) The complex conjugate of $\Psi(x, t)$ is

$$\Psi^*(x, t) = A^* e^{-i(k_1 x - \omega_1 t)} + A^* e^{-i(k_2 x - \omega_2 t)}$$

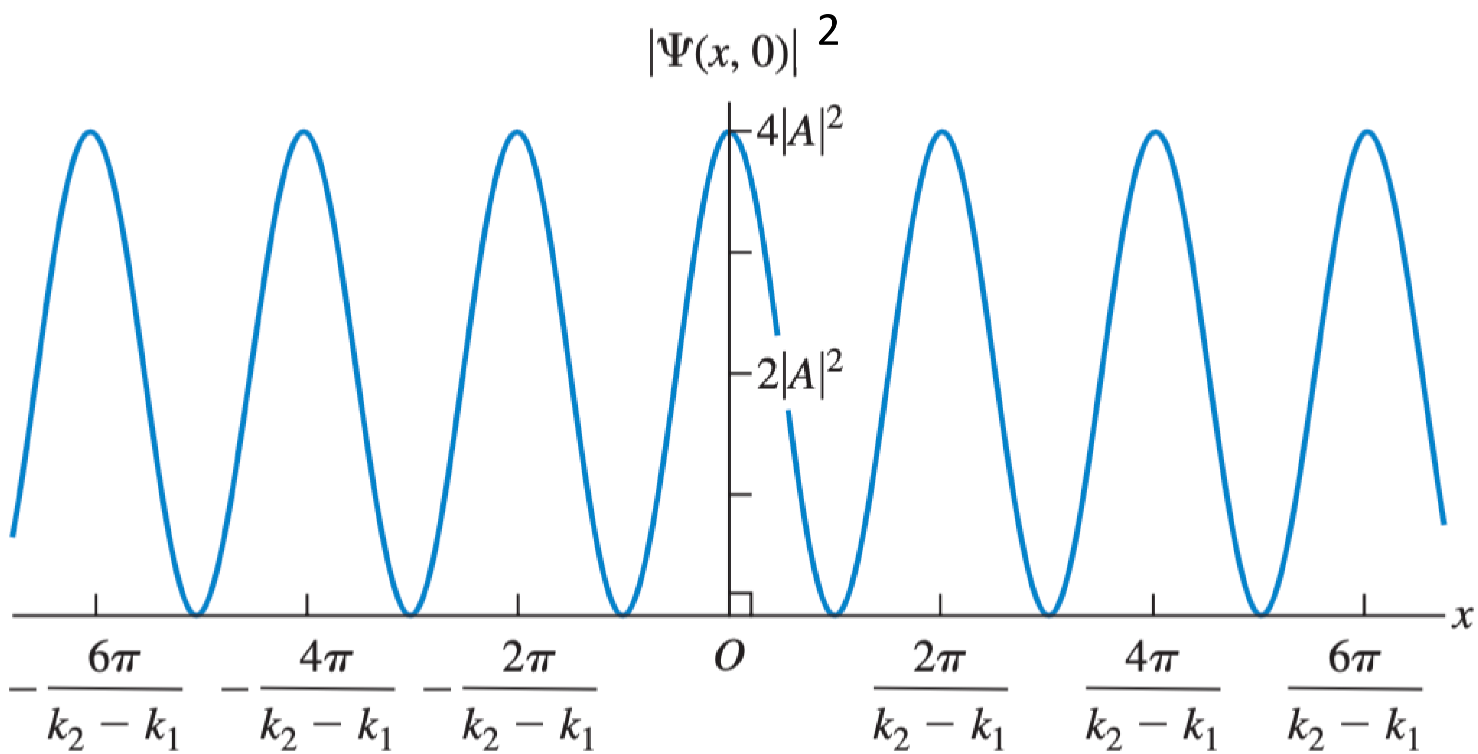
Hence

$$\begin{aligned}
&|\Psi(x, t)|^2 \\
&\quad = \Psi^*(x, t)\Psi(x, t) \\
&\quad = \left(A^* e^{-i(k_1 x - \omega_1 t)} + A^* e^{-i(k_2 x - \omega_2 t)}\right)\left(A e^{i(k_1 x - \omega_1 t)} + A e^{i(k_2 x - \omega_2 t)}\right) \\
&\quad = A^* A \left[\begin{array}{l} e^{-i(k_1 x - \omega_1 t)} e^{i(k_1 x - \omega_1 t)} + e^{-i(k_2 x - \omega_2 t)} e^{i(k_2 x - \omega_2 t)} \\ \qquad + e^{-i(k_1 x - \omega_1 t)} e^{i(k_2 x - \omega_2 t)} + e^{-i(k_2 x - \omega_2 t)} e^{i(k_1 x - \omega_1 t)} \end{array}\right] \\
&\quad = |A|^2 \left[e^0 + e^0 + e^{i[(k_2 - k_1)x - (\omega_2 - \omega_1)t]} + e^{-i[(k_2 - k_1)x - (\omega_2 - \omega_1)t]}\right]
\end{aligned}$$

To simplify this expression, recall that $e^0 = 1$. From Euler's formula, $e^{i\theta} = \cos\theta + i\sin\theta$ and $e^{-i\theta} = \cos\theta - i\sin\theta$, so $e^{i\theta} + e^{-i\theta} = 2\cos\theta$. Hence

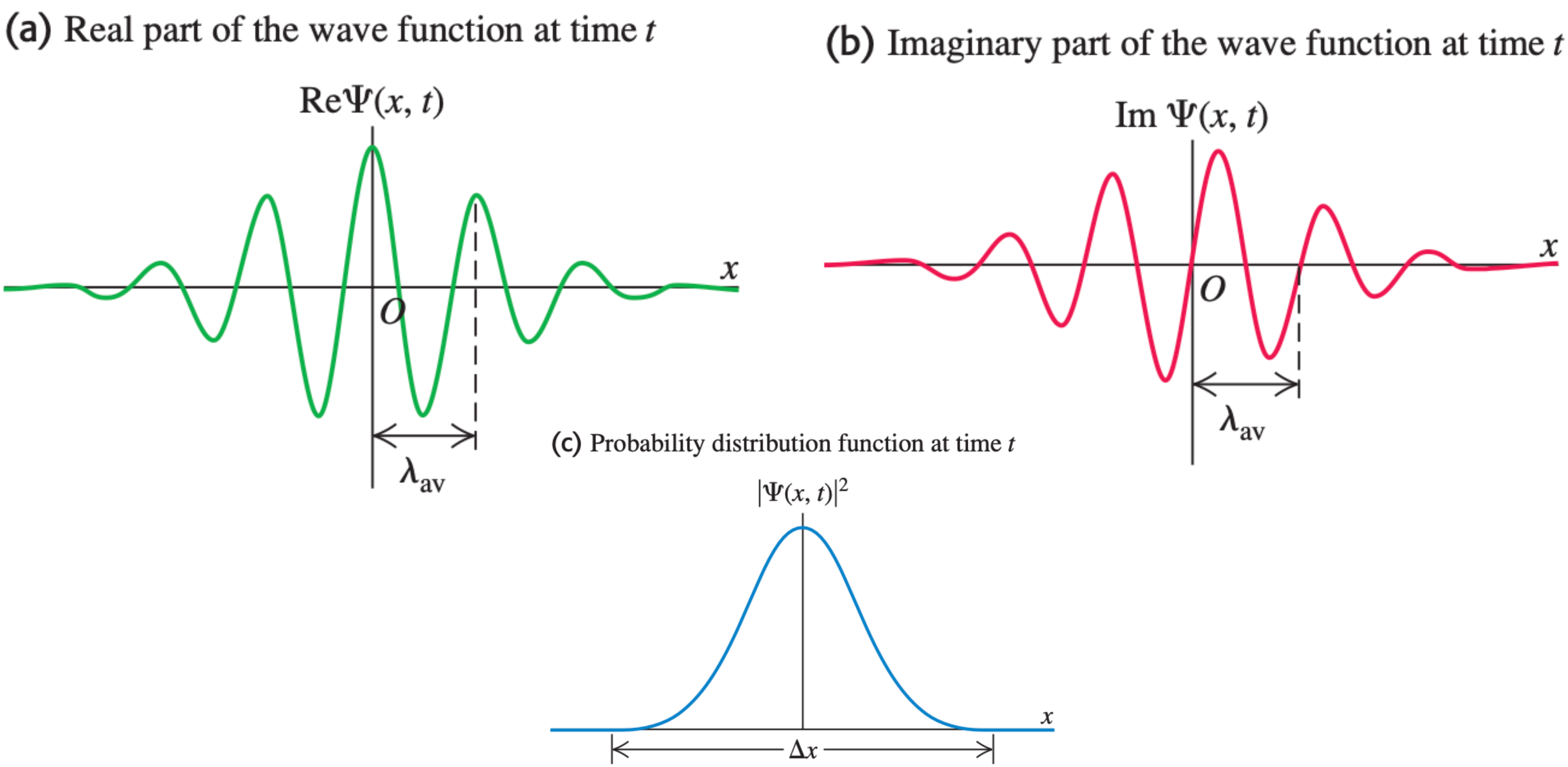
$$\begin{aligned}
|\Psi(x, t)|^2 &= |A|^2\{2 + 2\cos[(k_2 - k_1)x - (\omega_2 - \omega_1)t]\} \\
&= 2|A|^2\{1 + \cos[(k_2 - k_1)x - (\omega_2 - \omega_1)t]\}
\end{aligned}$$

Sample Problem



40-1 Wave Functions and the One-Dimensional Schrodinger Equation

Wave packet / wave pulse with wavelength $\lambda_{av} = 2\pi/k_{av}$



40-1 Wave Functions and the One-Dimensional Schrodinger Equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$ (general one-dimensional Schrödinger equation)

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$$ (time-dependent wave function for a state of definite energy)

40-1 Wave Functions and the One-Dimensional Schrodinger Equation

$$\Psi(x, t) = \psi(x)e^{-iEt/\hbar}$$ (time-dependent wave function for a state of definite energy)

$$-\frac{\hbar^2}{2m}\frac{\partial^2[\psi(x)e^{-iEt/\hbar}]}{\partial x^2} + U(x)\psi(x)e^{-iEt/\hbar} = i\hbar\frac{\partial[\psi(x)e^{-iEt/\hbar}]}{\partial t}$$

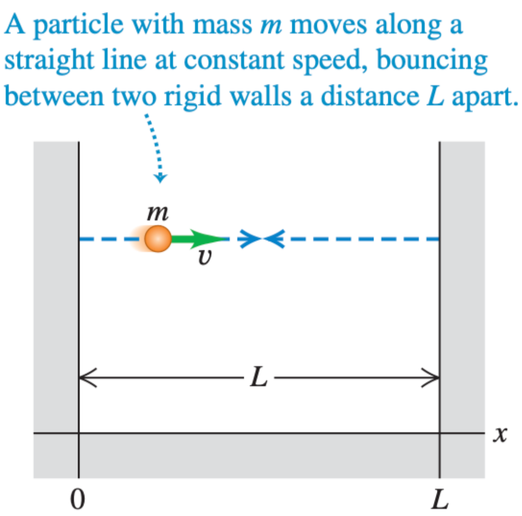
$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}e^{-iEt/\hbar} + U(x)\psi(x)e^{-iEt/\hbar} = i\hbar\left(\frac{-iE}{\hbar}\right)[\psi(x)e^{-iEt/\hbar}]$$

$$= E\psi(x)e^{-iEt/\hbar}$$

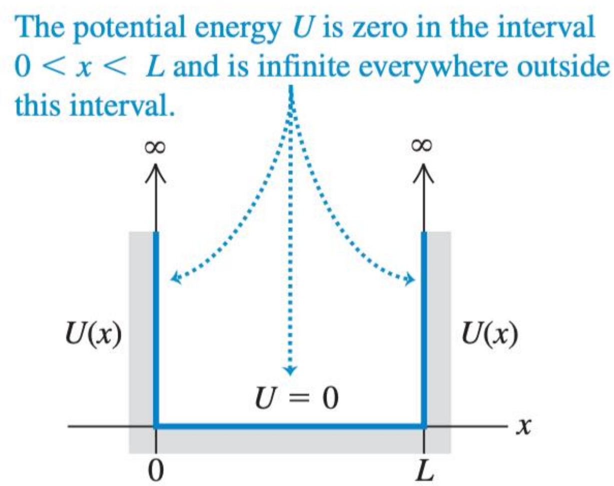
$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x)$$ (time-independent Schrödinger equation)

40-2 Particle in a Box

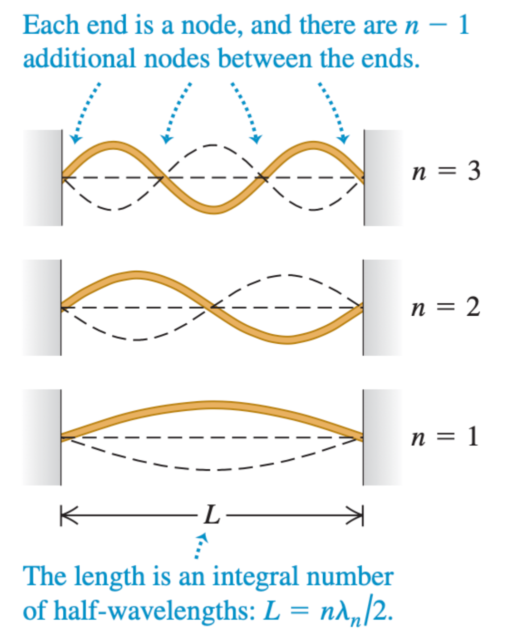
40.8 The Newtonian view of a particle in a box.



40.9 The potential-energy function for a particle in a box.



40.10 Normal modes of vibration for a string with length L, held at both ends.



40-2 Particle in a Box

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \qquad \text{(particle in a box)}$$

boundary conditions $\quad \psi(x)$ must be zero

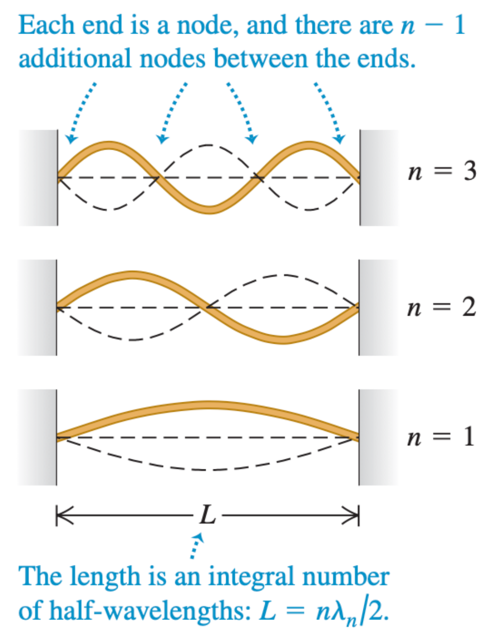
at $x = 0$ and $x = L$

$$\psi(x) = 2iA_1 \sin kx = C \sin kx$$

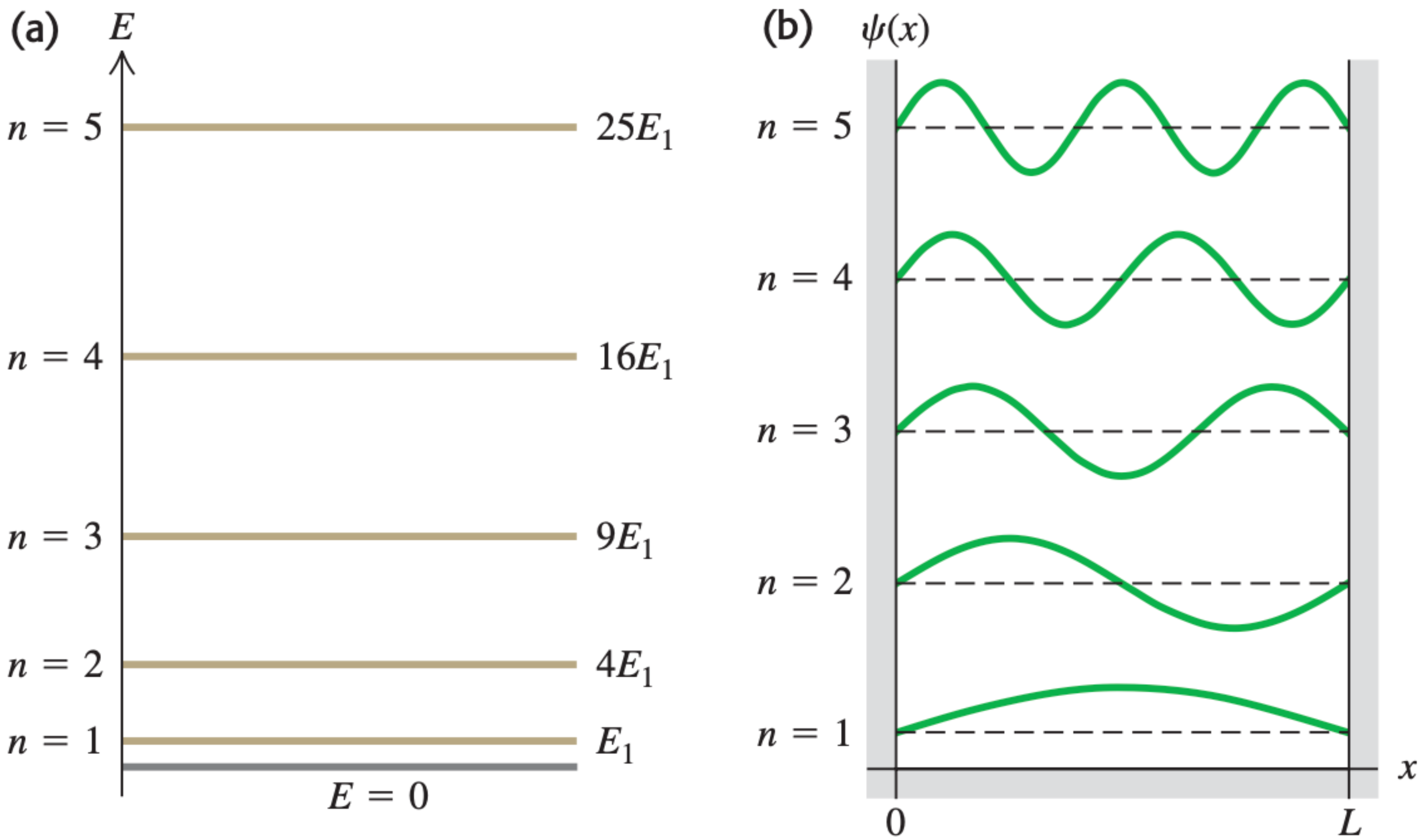
$$k = \frac{n\pi}{L} \quad \text{and} \quad \lambda = \frac{2\pi}{k} = \frac{2L}{n} \quad (n = 1, 2, 3, \ldots)$$

$$E_n = \frac{{p_n}^2}{2m} = \frac{n^2h^2}{8mL^2} = \frac{n^2\pi^2\hbar^2}{2mL^2} \quad (n = 1, 2, 3, \ldots)$$

40.10 Normal modes of vibration for a string with length L, held at both ends.



40-2 Particle in a Box



Sample Problem

Example 40.3 **Electron in an atom-size box**

Find the first two energy levels for an electron confined to a one-dimensional box 5.0×10^{-10} m across (about the diameter of an atom).

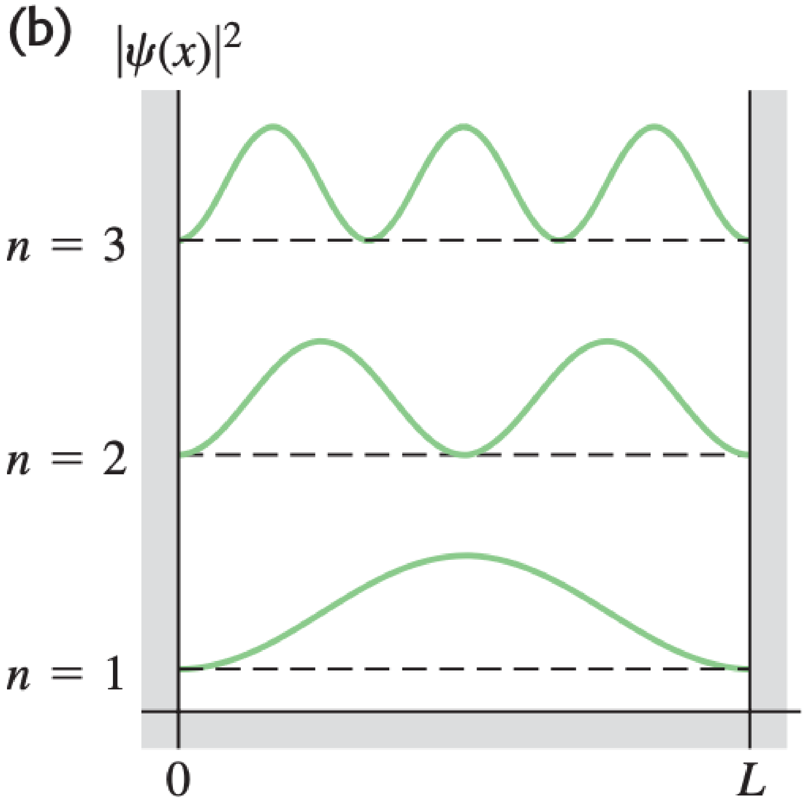
EXECUTE: From Eq. (40.31),

$$E_1 = \frac{h^2}{8mL^2} = \frac{(6.626 \times 10^{-34}\ \mathrm{J \cdot s})^2}{8(9.109 \times 10^{-31}\ \mathrm{kg})(5.0 \times 10^{-10}\ \mathrm{m})^2}$$

$$= 2.4 \times 10^{-19}\ \mathrm{J} = 1.5\ \mathrm{eV}$$

$$E_2 = \frac{2^2 h^2}{8mL^2} = 4E_1 = 9.6 \times 10^{-19}\ \mathrm{J} = 6.0\ \mathrm{eV}$$

40-2 Particle in a Box



Normalization

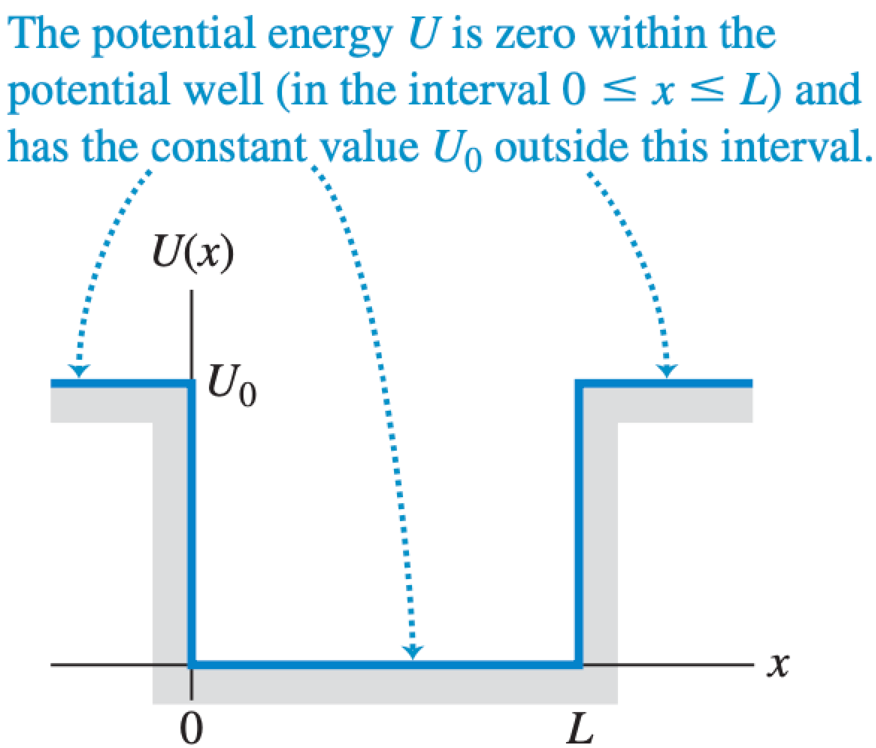
$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1$$

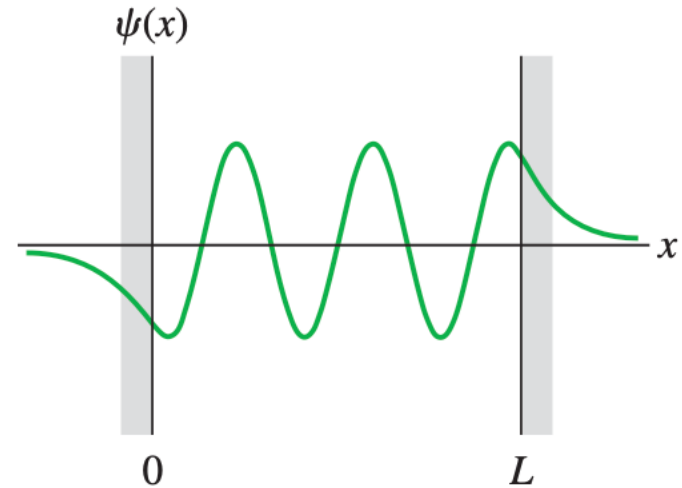
$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L} \quad (n = 1, 2, 3, \ldots)$$

Time dependence

$$\Psi_n(x, t) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) e^{-iE_n t/\hbar}$$

40-3 Potential Wells





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

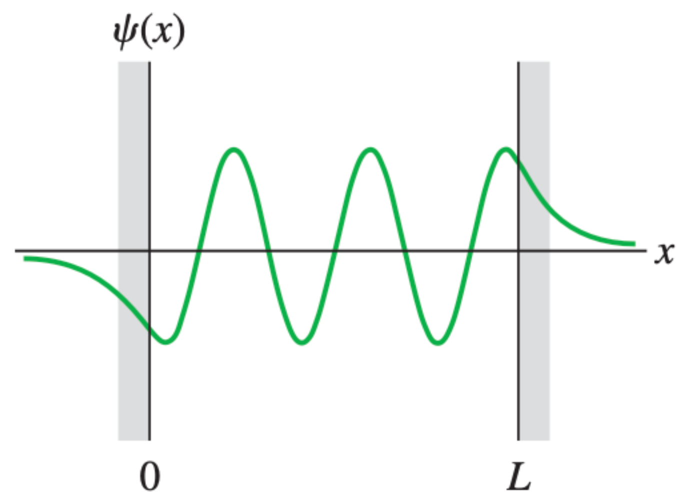
$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U_0\psi(x) = E\psi(x)$$

40-3 Potential Wells

inside the well

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

$$\psi(x) = A\cos\left(\frac{\sqrt{2mE}}{\hbar}x\right) + B\sin\left(\frac{\sqrt{2mE}}{\hbar}x\right)$$



outside the well

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U_0\psi(x) = E\psi(x)$$

$$\psi(x) = Ce^{\kappa x} + De^{-\kappa x}$$

Sample Problem

Example 40.5 **Outside a finite well**

(a) Show that Eq. (40.40), $\psi(x) = Ce^{\kappa x} + De^{-\kappa x}$, is indeed a solution of the time-independent Schrödinger equation outside a finite well of height U_0. (b) What happens to $\psi(x)$ in the limit $U_0 \to \infty$?

EXECUTE: (a) We must show that $\psi(x) = Ce^{\kappa x} + De^{-\kappa x}$ satisfies $d^2\psi(x)/dx^2 = [2m(U_0 - E)/\hbar^2]\psi(x)$. We recall that $(d/du)e^{au} = ae^{au}$ and $(d^2/du^2)e^{au} = a^2e^{au}$; the left-hand side of the Schrödinger equation is then

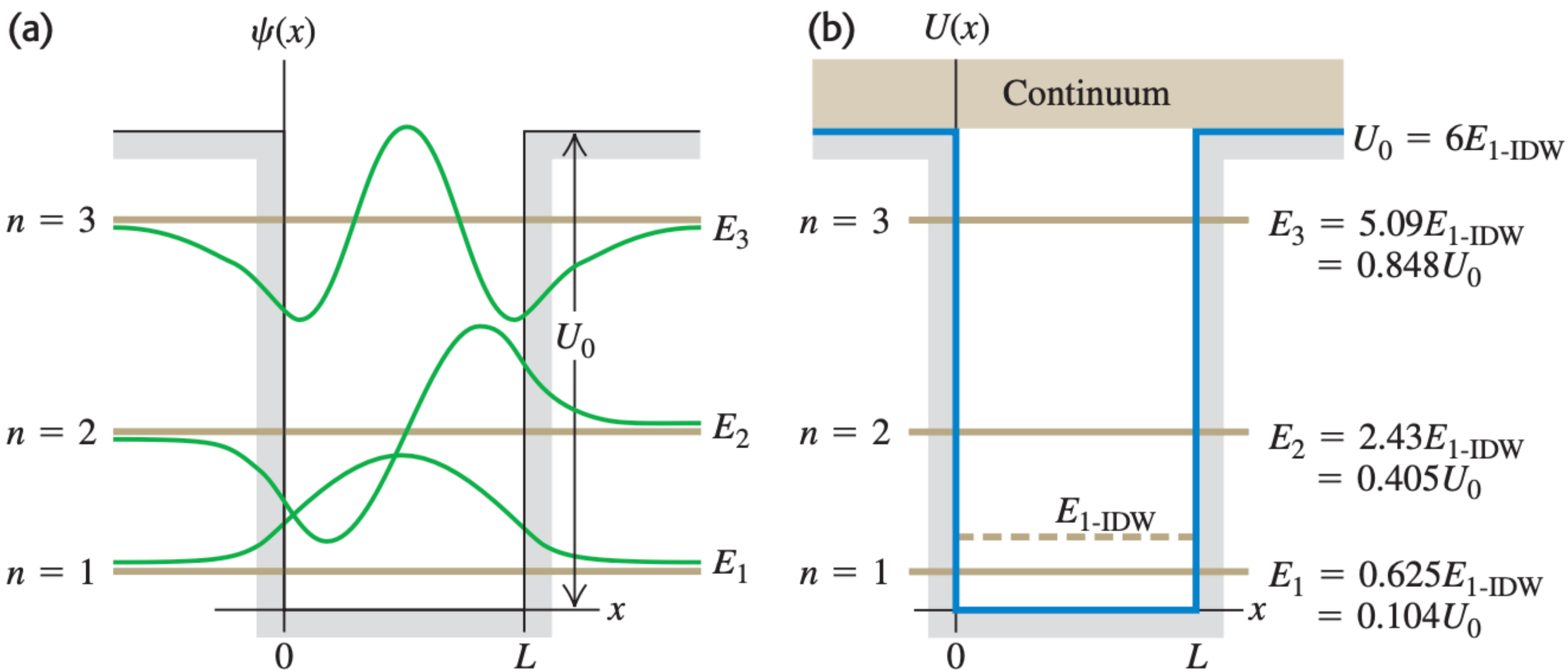
$$\begin{aligned}\frac{d^2\psi(x)}{dx^2} &= \frac{d^2}{dx^2}(Ce^{\kappa x}) + \frac{d^2}{dx^2}(De^{-\kappa x}) \\ &= C\kappa^2 e^{\kappa x} + D(-\kappa)^2 e^{-\kappa x} \\ &= \kappa^2(Ce^{\kappa x} + De^{-\kappa x}) \\ &= \kappa^2\psi(x)\end{aligned}$$

Since from Eq. (40.40) $\kappa^2 = 2m(U_0 - E)/\hbar^2$, this is equal to the right-hand side of the equation. The equation is satisfied, and $\psi(x)$ is a solution.

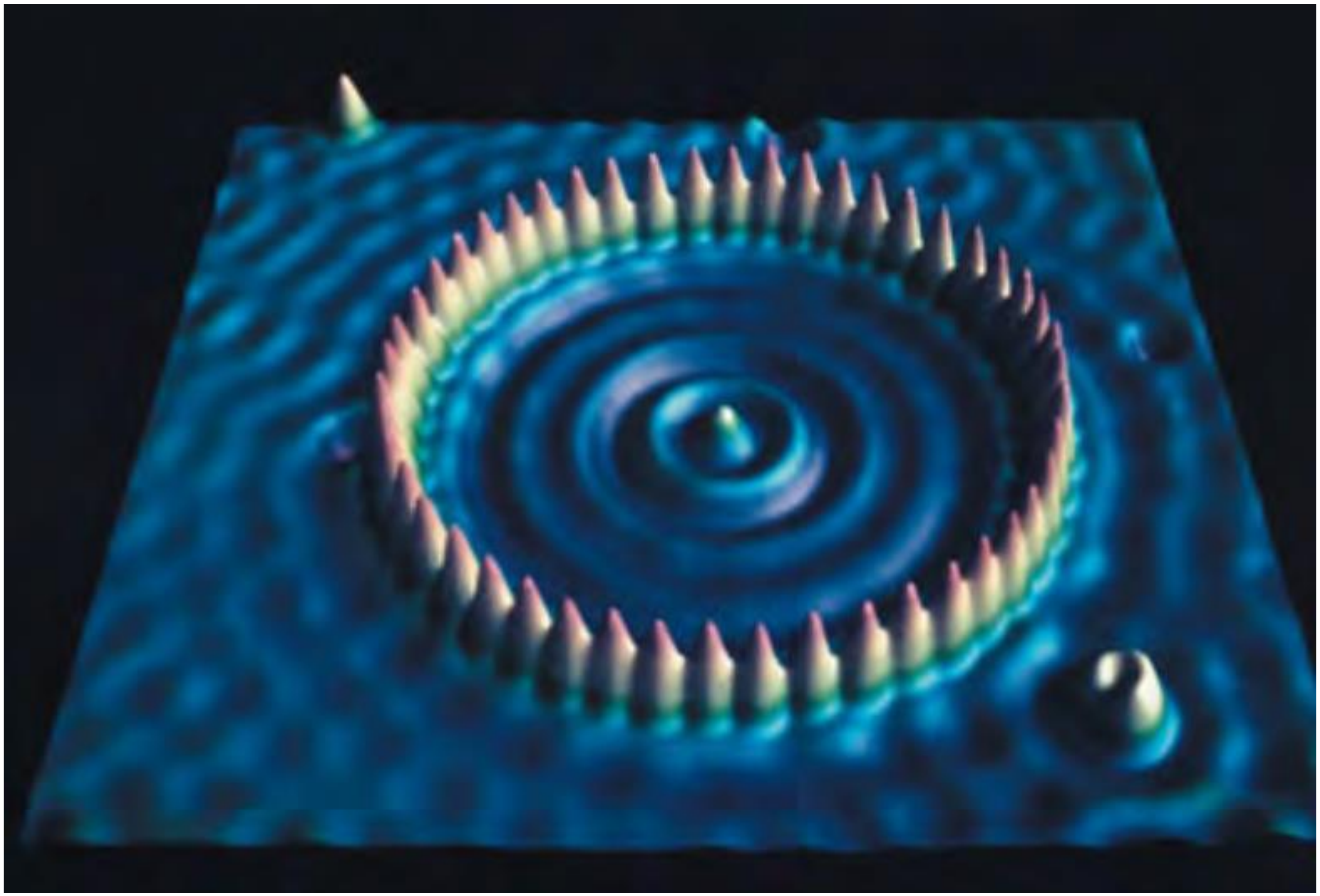
(b) As U_0 approaches infinity, κ also approaches infinity. In the region $x < 0$, $\psi(x) = Ce^{\kappa x}$; as $\kappa \to \infty$, $\kappa x \to -\infty$ (since x is negative) and $e^{\kappa x} \to 0$, so the wave function approaches zero for all $x < 0$. Likewise, we can show that the wave function also approaches zero for all $x > L$. This is just what we found in Section 40.2; the wave function for a particle in a box must be zero outside the box.

40-3 Potential Wells

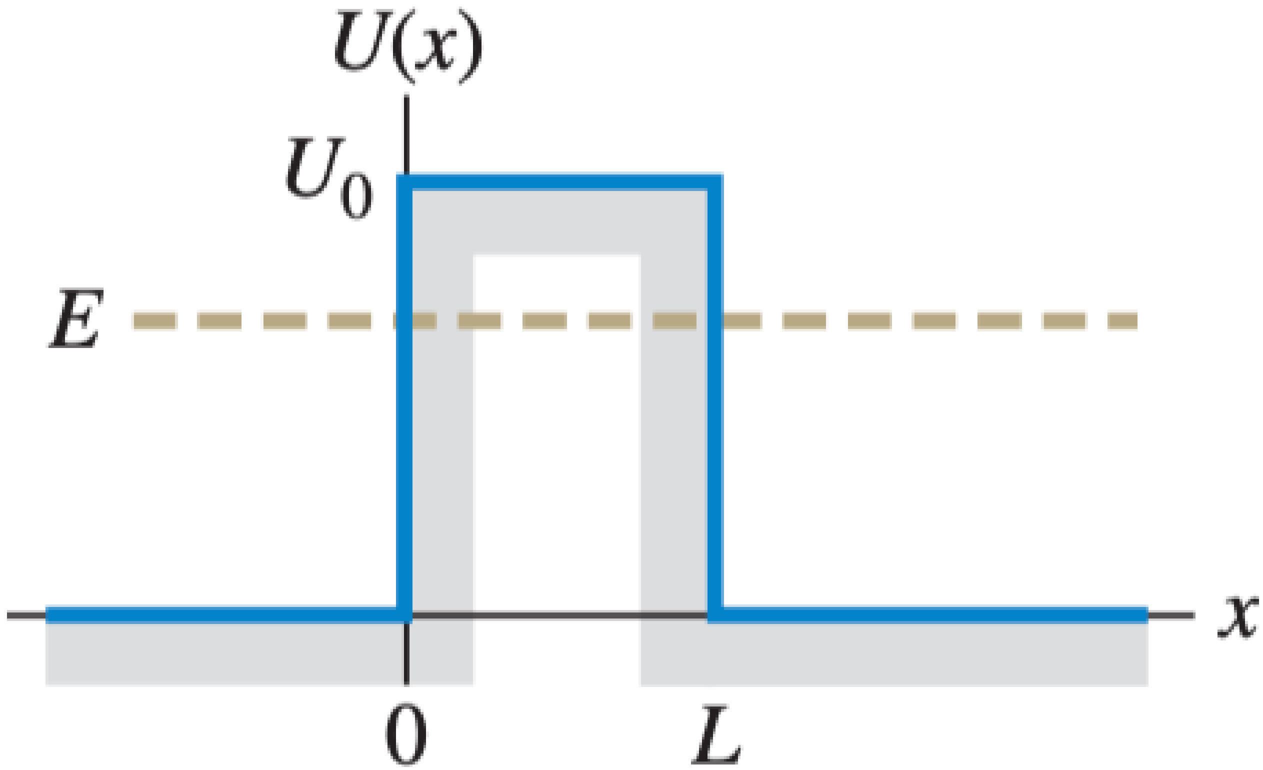
Comparing Finite and Infinite Square Wells



40-3 Potential Wells



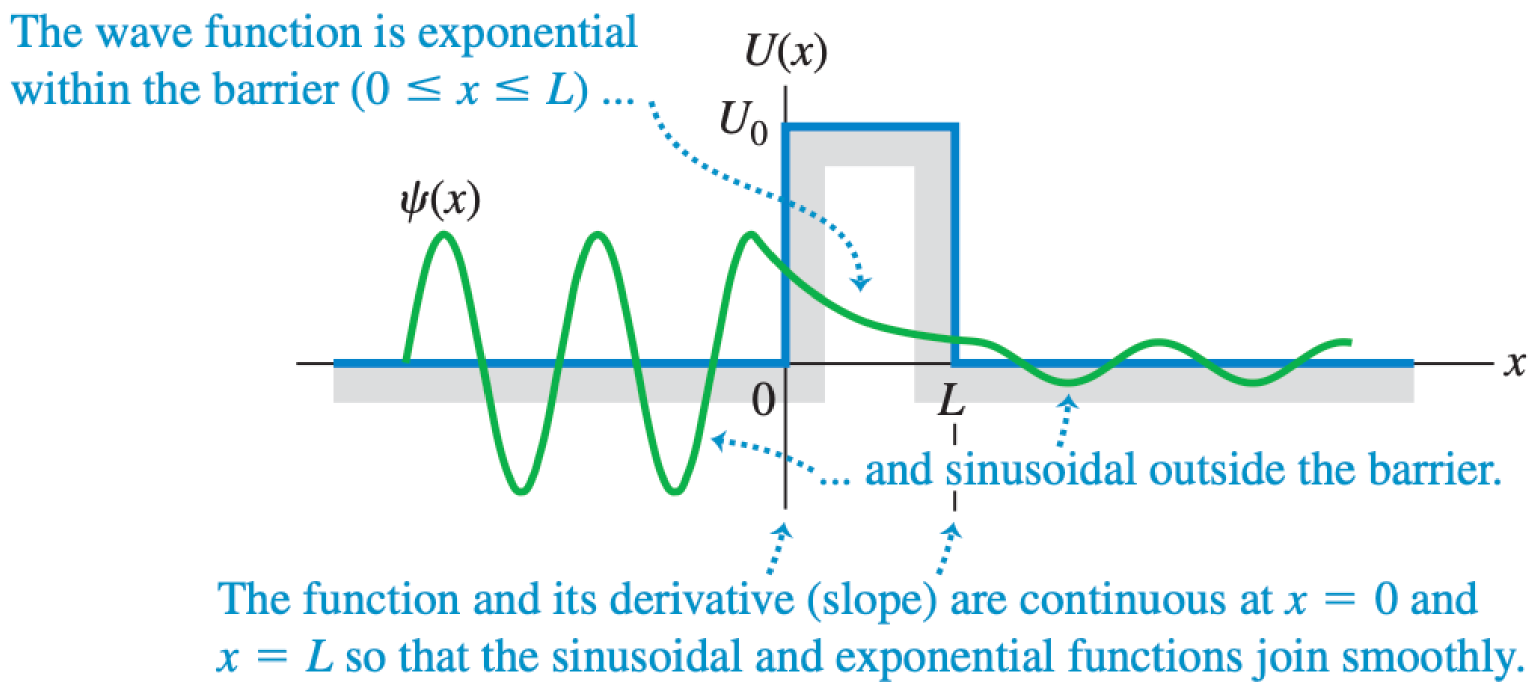
40-4 Potential Barriers and Tunneling



Newtonian mechanics?

The particle with energy E can’t pass over the barrier

40-4 Potential Barriers and Tunneling



$$T = Ge^{-2\kappa L} \text{ where } G = 16\frac{E}{U_0}\left(1 - \frac{E}{U_0}\right) \text{ and } \kappa = \frac{\sqrt{2m(U_0 - E)}}{\hbar}$$

(probability of tunneling)

Sample Problem

Example 40.7 **Tunneling through a barrier**

A 2.0-eV electron encounters a barrier 5.0 eV high. What is the probability that it will tunnel through the barrier if the barrier width is (a) 1.00 nm and (b) 0.50 nm?

EXECUTE: First we evaluate G and κ in Eq. (40.42), using $E = 2.0\ \text{eV}$:

$$G = 16\left(\frac{2.0\ \text{eV}}{5.0\ \text{eV}}\right)\left(1 - \frac{2.0\ \text{eV}}{5.0\ \text{eV}}\right) = 3.8$$

$$U_0 - E = 5.0\ \text{eV} - 2.0\ \text{eV} = 3.0\ \text{eV} = 4.8 \times 10^{-19}\ \text{J}$$

$$\kappa = \frac{\sqrt{2(9.11 \times 10^{-31}\ \text{kg})(4.8 \times 10^{-19}\ \text{J})}}{1.055 \times 10^{-34}\ \text{J} \cdot \text{s}} = 8.9 \times 10^{9}\ \text{m}^{-1}$$

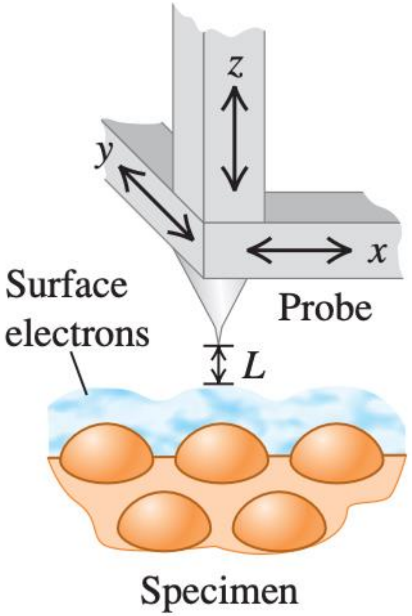
(a) When $L = 1.00\ \text{nm} = 1.00 \times 10^{-9}\ \text{m}$, $2\kappa L = 2(8.9 \times 10^{9}\ \text{m}^{-1})(1.00 \times 10^{-9}\ \text{m}) = 17.8$ and $T = Ge^{-2\kappa L} = 3.8e^{-17.8} = 7.1 \times 10^{-8}$.

(b) When $L = 0.50\ \text{nm}$, one-half of 1.00 nm, $2\kappa L$ is one-half of 17.8, or 8.9. Hence $T = 3.8e^{-8.9} = 5.2 \times 10^{-4}$.

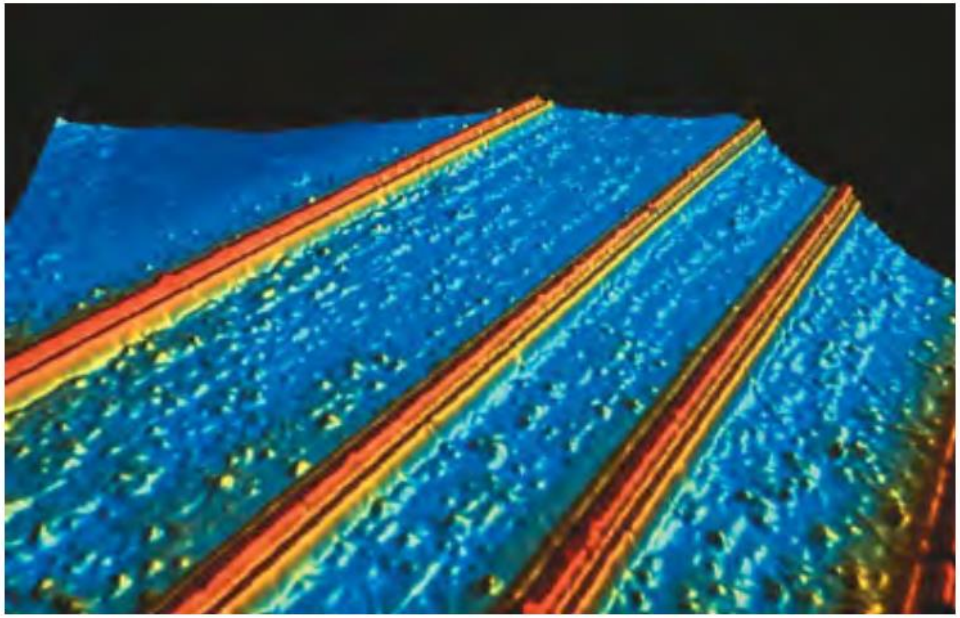
40-4 Potential Barriers and Tunneling

Scanning tunneling microscope (STM)

(a)



(b)



40-4 Potential Barriers and Tunneling

Application Electron Tunneling in Enzymes

Protein molecules play essential roles as enzymes in living organisms. Enzymes like the one shown here are large molecules, and in many cases their function depends on the ability of electrons to tunnel across the space that separates one part of the molecule from another. Without tunneling, life as we know it would be impossible!