Chapter 41

1D Wavefunctions

Chapter 41. One-Dimensional Quantum Mechanics

Topics:

- Schrödinger's Equation: The Law of Psi
- Solving the Schrödinger Equation
- A Particle in a Rigid Box: Energies and Wave Functions
- A Particle in a Rigid Box: Interpreting the Solution
- The Correspondence Principle
- Finite Potential Wells
- Wave-Function Shapes
- The Quantum Harmonic Oscillator
- More Quantum Models
- Quantum-Mechanical Tunneling

The wave function is complex.

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + U(x)\psi(x,t)$$

What is the PDF for finding a particle at x ?

$$P(x,t) = \left|\psi(x,t)\right|^2$$

Step 1: solve Schrodinger equation for wave function

Step 2: probability of finding particle at x is $P(x,t) = \left|\psi(x,t)\right|^2$

Stationary States - Bohr Hypothesis

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + U(x)\psi(x,t)$$

$$\psi(x,t) = \hat{\psi}(x)e^{-1Et/\hbar} \qquad \omega = \frac{E}{\hbar}$$

Stationary State satisfies

$$E\hat{\psi}(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\hat{\psi}(x) + U(x)\hat{\psi}(x)$$

Stationary states

$$E\hat{\psi}(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\hat{\psi}(x) + U(x)\hat{\psi}(x)$$

Rewriting:

$$\frac{\partial^2}{\partial x^2}\hat{\psi}(x) = -\beta^2(x)\hat{\psi}(x)$$

$$\beta^2(x) = \frac{2m}{\hbar^2}\left(E - U(x)\right)$$

Dependence on x comes from dependence on potential

$$\frac{\partial^2}{\partial x^2}\hat{\psi}(x) = -\beta^2(x)\hat{\psi}(x)$$

$$\beta^2(x) = \frac{2m}{\hbar^2}\left(E - U(x)\right)$$

Classically

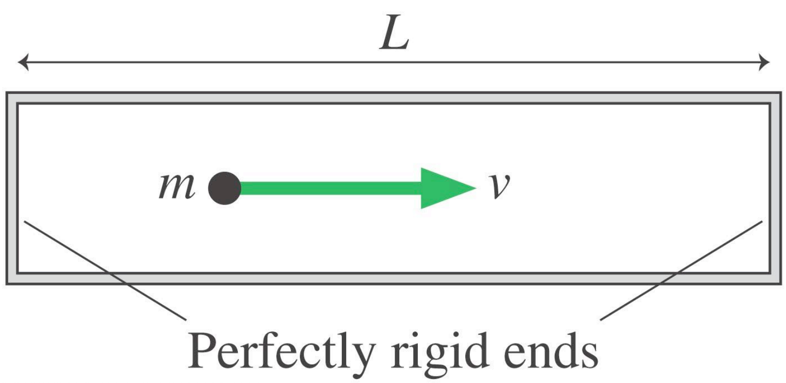
$$\left(E - U(x)\right) = K$$

K= kinetic energy

Requirements on wave function

1. Wave function is continuous
2. Wave function is normalizable

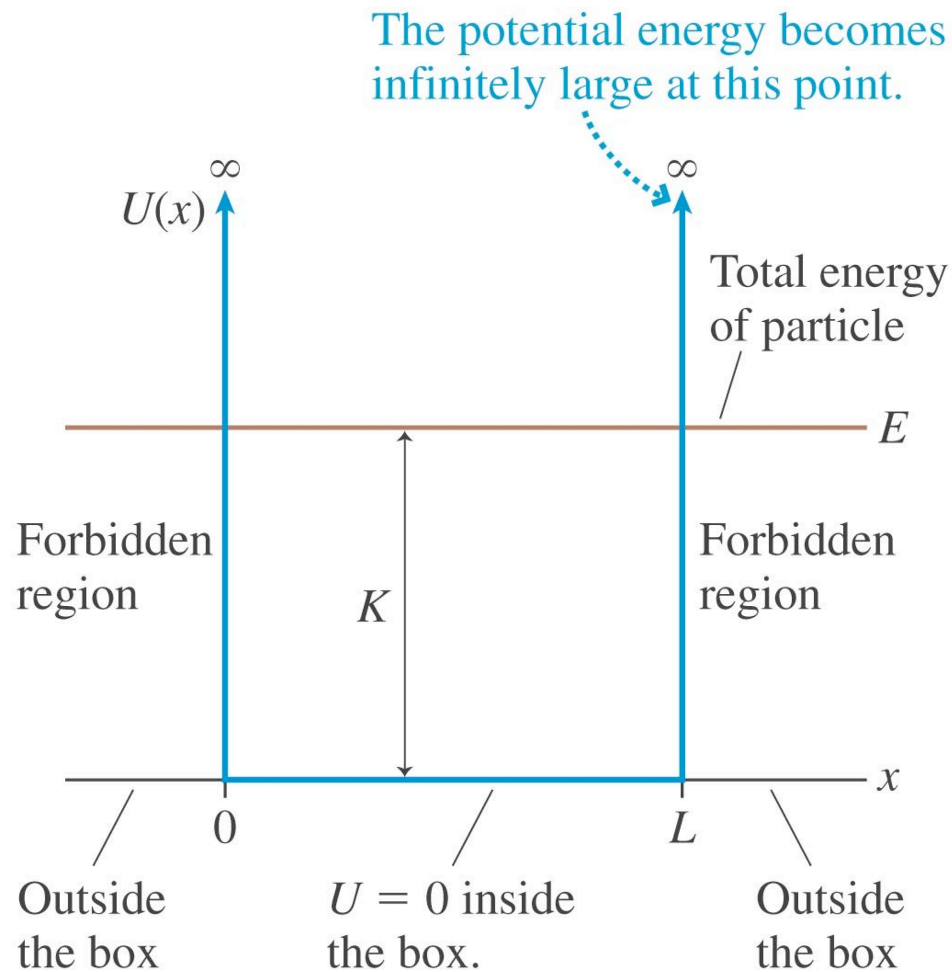
$$\int_{-\infty} P(x)\,dx = \int_{-\infty} |\psi(x)|^2 dx = 1$$



$$\frac{\partial^2}{\partial x^2}\hat{\psi}(x) = -\beta^2(x)\hat{\psi}(x)$$

$$\beta^2(x) = \frac{2m}{\hbar^2}\left(E - U(x)\right)$$

$$\beta^2(x) = \frac{2m}{\hbar^2}(K)$$



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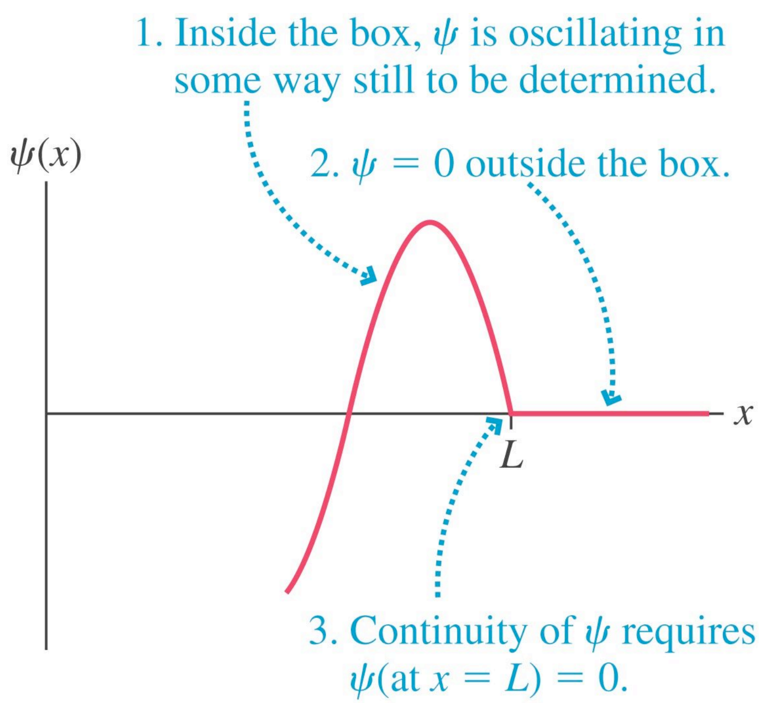
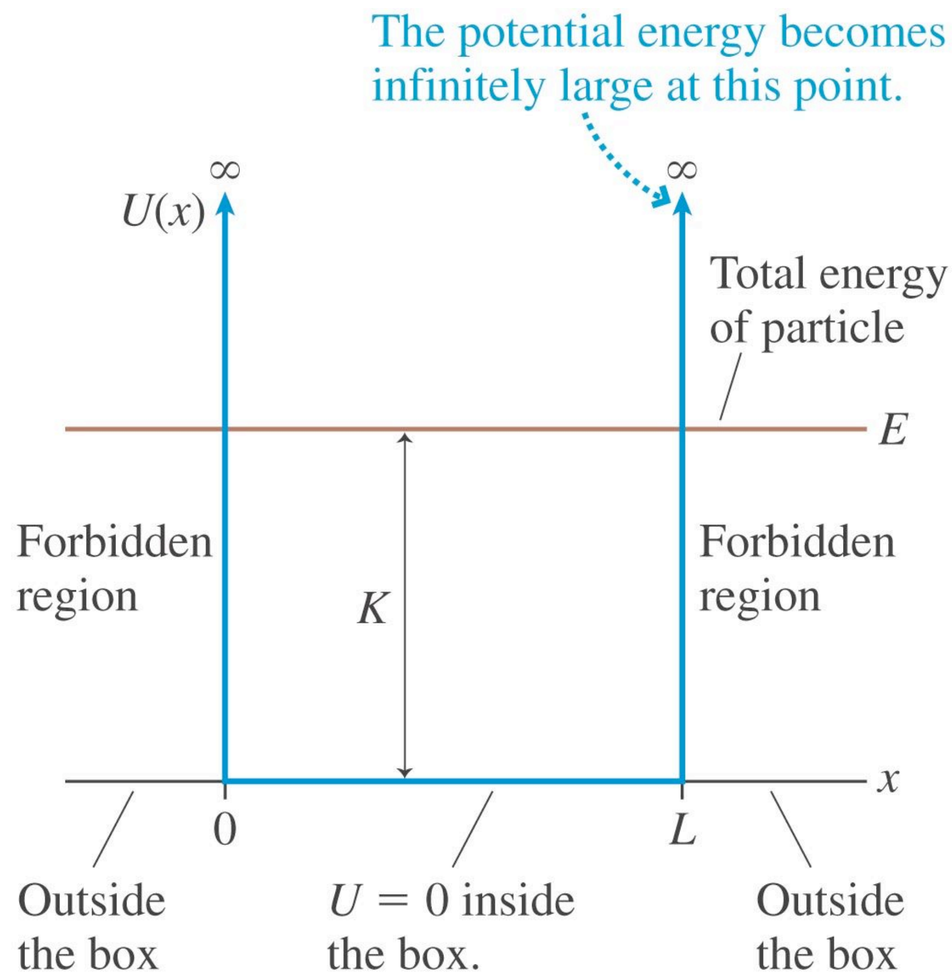




For $0<x<L$

$$\frac{\partial^2}{\partial x^2}\hat{\psi}(x) = -\beta^2\hat{\psi}(x)$$

Solution:

$$\hat{\psi}(x) = A\sin\beta x + B\cos\beta x$$

Boundary Conditions: $\hat{\psi}(0) = 0$ $\hat{\psi}(L) = 0$

$\hat{\psi}(0) = 0$ $\hat{\psi}(0) = A\sin 0 + B\cos 0 = B \rightarrow B = 0$

$\hat{\psi}(L) = 0$ $\hat{\psi}(L) = A\sin\beta L = 0$ $\beta L = n\pi$

$$\beta_n^{\ 2} = \frac{2m}{\hbar^2}\left(E_n\right)$$

Must have

$$E_n = \frac{\hbar^2}{2m}\beta_n^{\ 2} = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$ Energy is Quantized

A Particle in a Rigid Box

The solutions to the Schrödinger equation for a particle in a rigid box are

$$\psi_n(x) = A \sin \beta_n x = A \sin\left(\frac{n\pi x}{L}\right) \qquad n = 1, 2, 3, \ldots$$

$$\beta_n = \frac{\sqrt{2mE_n}}{\hbar} = \frac{n\pi}{L} \qquad n = 1, 2, 3, \ldots$$

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} = n^2 \frac{h^2}{8mL^2} \qquad n = 1, 2, 3, \ldots$$

For a particle in a box**, these energies are the only values of *E* for which there are physically meaningful solutions to the Schrödinger equation.** The particle's energy is quantized.

A Particle in a Rigid Box

The normalization condition, which we found in Chapter 40, is

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

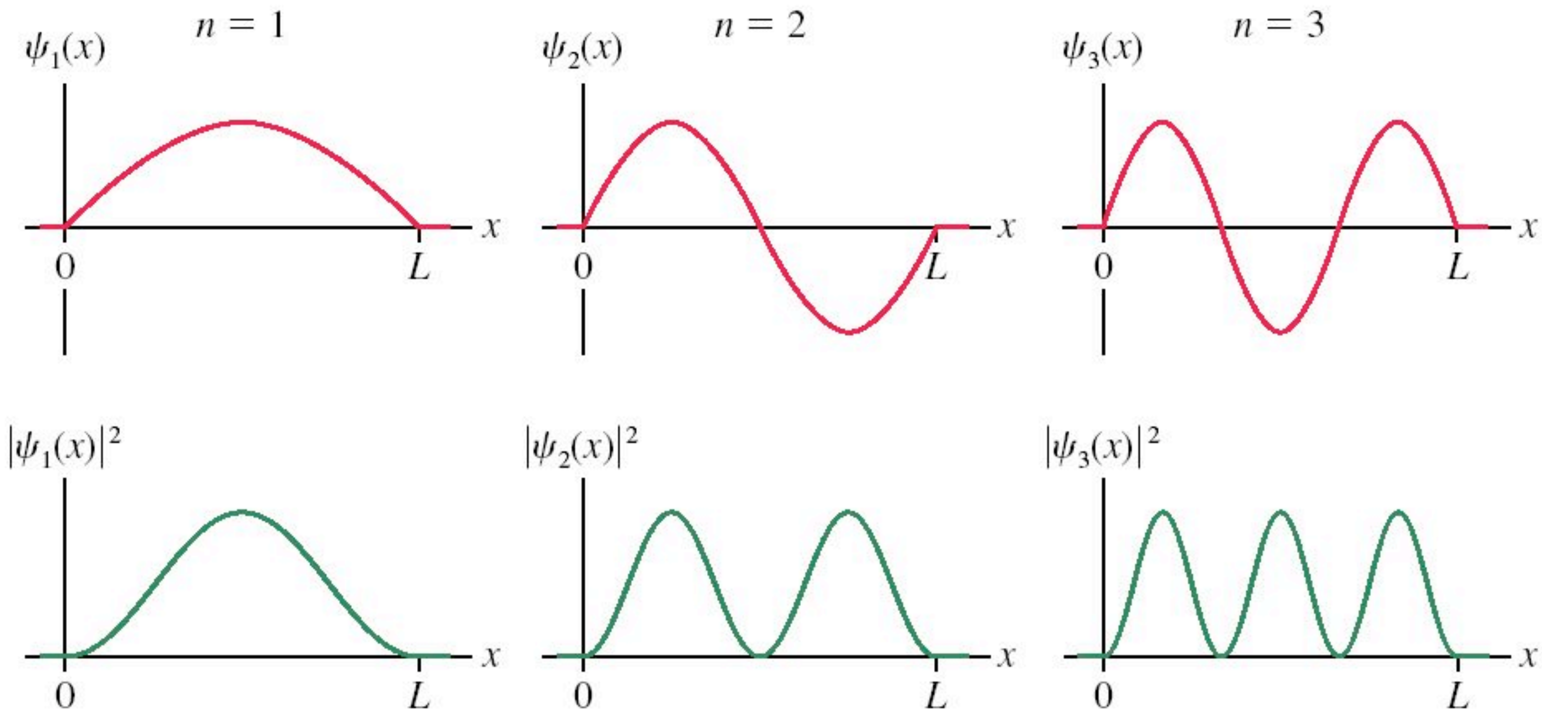
This condition determines the constants *A*:

$$A_n = \sqrt{\frac{2}{L}} \qquad n = 1, 2, 3, \ldots$$

The normalized wave function for the particle in quantum state *n* is

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) & 0 \le x \le L \\ 0 & x < 0 \text{ and } x > L \end{cases}$$

FIGURE 41.7 Wave functions and probability densities for a particle in a rigid box of length L.



EXAMPLE 41.2 Energy Levels and Quantum jumps

QUESTIONS:

EXAMPLE 41.2 Energy levels and quantum jumps

A semiconductor device known as a *quantum-well device* is designed to "trap" electrons in a 1.0-nm-wide region. Treat this as a one-dimensional problem.

a. What are the energies of the first three quantum states?
b. What wavelengths of light can these electrons absorb?

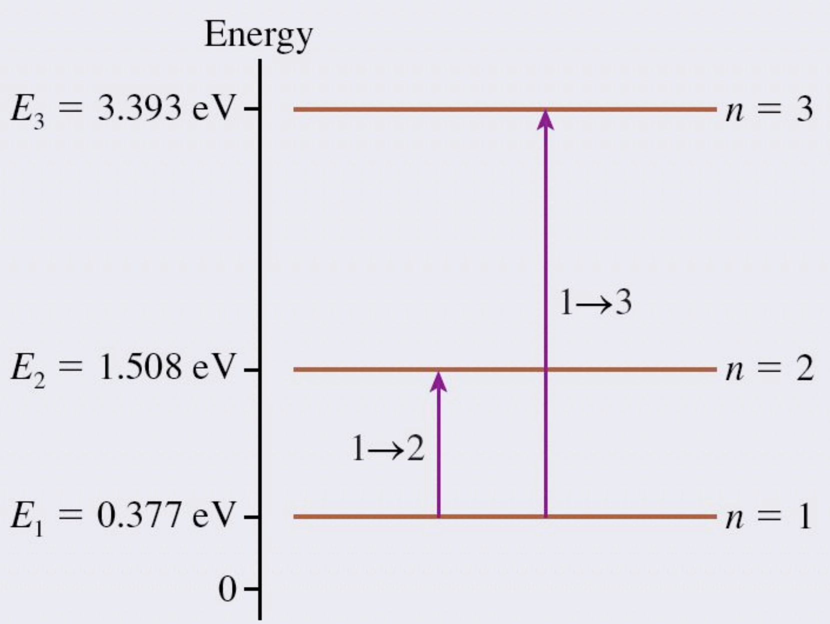
EXAMPLE 41.2 Energy Levels and Quantum jumps

MODEL Model an electron in a quantum-well device as a particle confined in a rigid box of length $L = 1.0$ nm.

EXAMPLE 41.2 Energy Levels and Quantum jumps

VISUALIZE **FIGURE 41.9** shows the first three energy levels and the transitions by which an electron in the ground state can absorb a photon.

FIGURE 41.9 Energy levels and quantum jumps for an electron in a quantum-well device.



EXAMPLE 41.2 Energy Levels and Quantum jumps

SOLVE a. The particle's mass is $m = m_e = 9.11 \times 10^{-31}$ kg. The allowed energies, in both J and eV, are

$$E_1 = \frac{h^2}{8mL^2} = 6.03 \times 10^{-20}\ \text{J} = 0.377\ \text{eV}$$

$$E_2 = 4E_1 = 1.508\ \text{eV}$$

$$E_3 = 9E_1 = 3.393\ \text{eV}$$

EXAMPLE 41.2 Energy Levels and Quantum jumps

b. An electron spends most of its time in the $n = 1$ ground state. According to Bohr's model of stationary states, the electron can absorb a photon of light and undergo a transition, or quantum jump, to $n = 2$ or $n = 3$ if the light has frequency $f = \Delta E/h$. The wavelengths, given by $\lambda = c/f = hc/\Delta E$, are

$$\lambda_{1\to2} = \frac{hc}{E_2 - E_1} = 1098 \text{ nm}$$

$$\lambda_{1\to3} = \frac{hc}{E_3 - E_1} = 411 \text{ nm}$$

EXAMPLE 41.2 Energy Levels and Quantum jumps

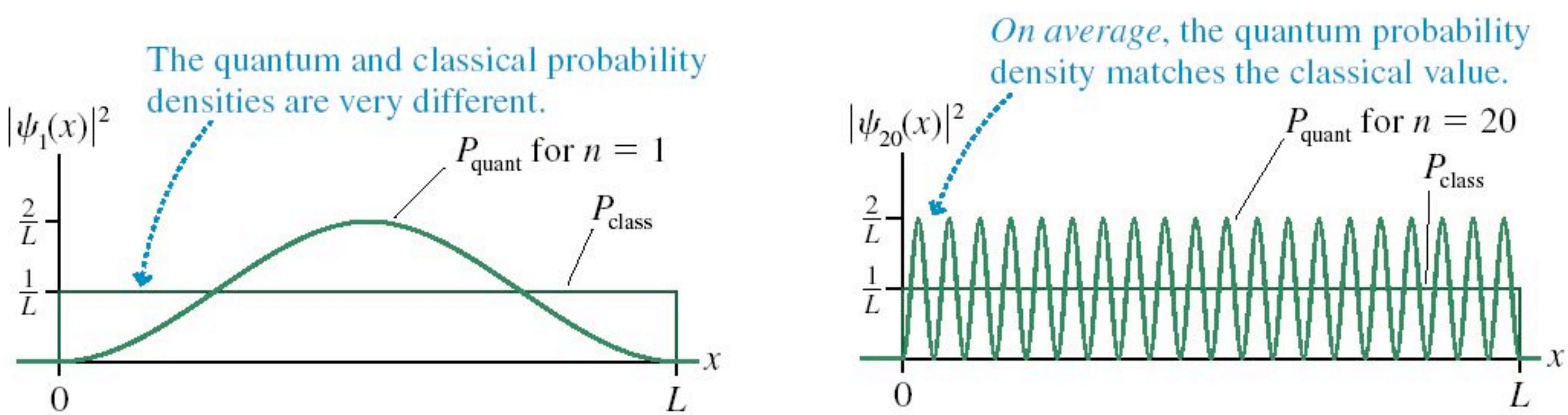
ASSESS In practice, various complications usually make the $1 \rightarrow 3$ transition unobservable. But quantum-well devices do indeed exhibit strong absorption and emission at the $\lambda_{1 \rightarrow 2}$ wavelength. In this example, which is typical of quantum-well devices, the wavelength is in the near-infrared portion of the spectrum. Devices such as these are used to construct the semiconductor lasers used in CD players and laser printers.

The Correspondence Principle

- Niels Bohr put forward the idea that the *average* behavior of a quantum system should begin to look like the classical solution in the limit that the quantum number becomes very large—that is, as $n \to \infty$.
- Because the radius of the Bohr hydrogen atom is $r = n^2 a_B$, the atom becomes a macroscopic object as n becomes very large.
- Bohr's idea, that the quantum world should blend smoothly into the classical world for high quantum numbers, is today known as the **correspondence principle.**

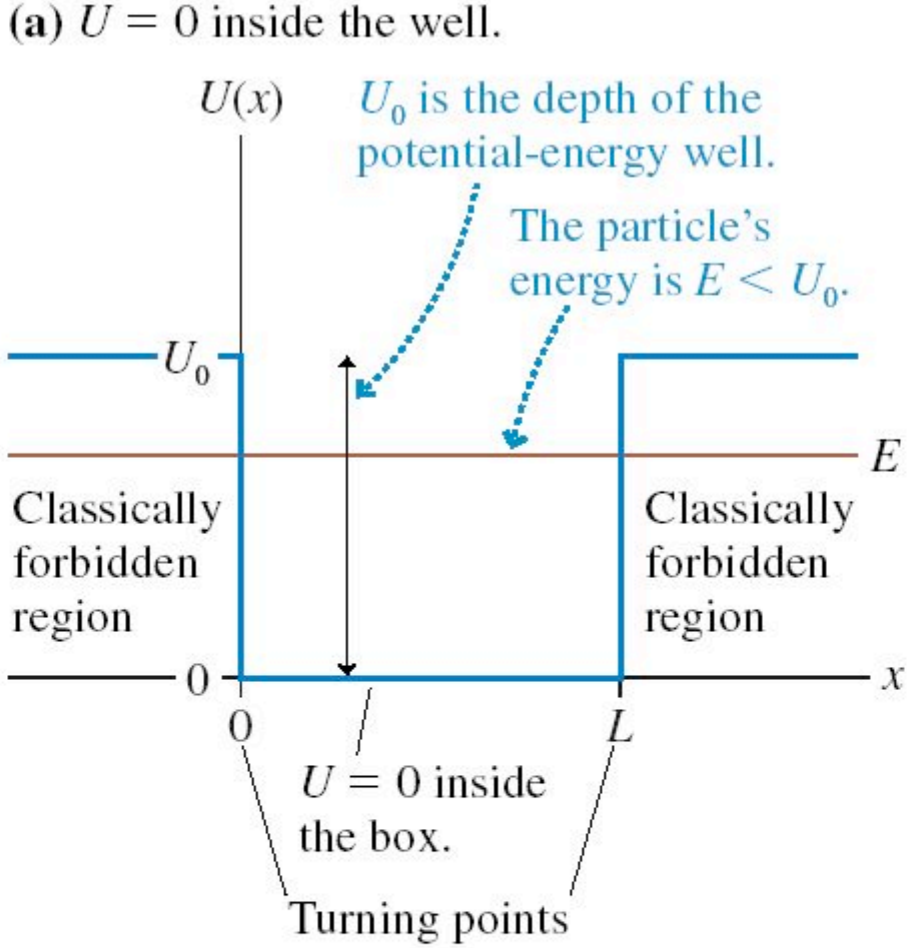
The Correspondence Principle

FIGURE 41.12 The quantum and classical probability densities for a particle in a box.



As n gets even bigger and the number of oscillations increases, the probability of finding the particle in an interval Δx will be the same for both the quantum and the classical particles as long as Δx is large enough to include several oscillations of the wave function. This is in agreement with Bohr’s correspondence principle.

FIGURE 41.13 A finite potential well of width L and depth U_0.



$$\frac{\partial^2}{\partial x^2}\hat{\psi}(x) = -\beta^2(x)\hat{\psi}(x)$$

$$\beta^2(x) = \frac{2m}{\hbar^2}\left(E - U(x)\right)$$

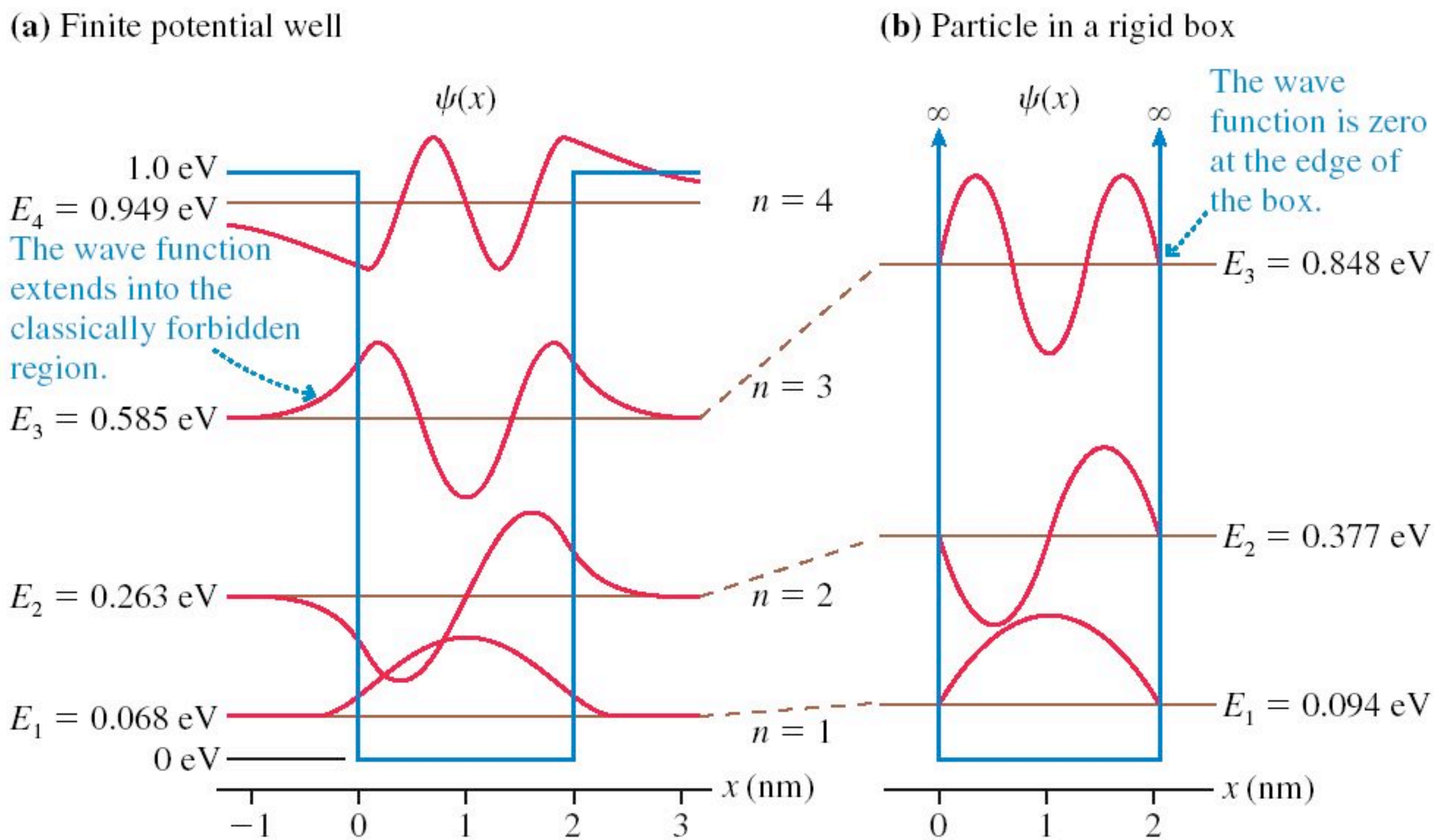
Between x=0 and x=L

$$\beta^2(x) > 0$$

Outside

$$\beta^2(x) < 0$$

FIGURE 41.14 Energy levels and wave functions for a finite potential well. For comparison, the energies and wave functions are shown for a rigid box of equal width.



Finite Potential Wells

The quantum-mechanical solution for a particle in a finite potential well has some important properties:

- The particle's energy is quantized.
- There are only a finite number of **bound states**. There are no stationary states with $E > U_0$ because such a particle would not remain in the well.
- The wave functions are qualitatively similar to those of a particle in a rigid box, but the energies are somewhat lower.
- The wave functions extend into the classically forbidden regions. (tunneling)

Finite Potential Wells

The wave function in the classically forbidden region of a finite potential well is

$$\psi(x) = \psi_{\text{edge}} e^{-(x-L)/\eta} \quad \text{for } x \geq L$$

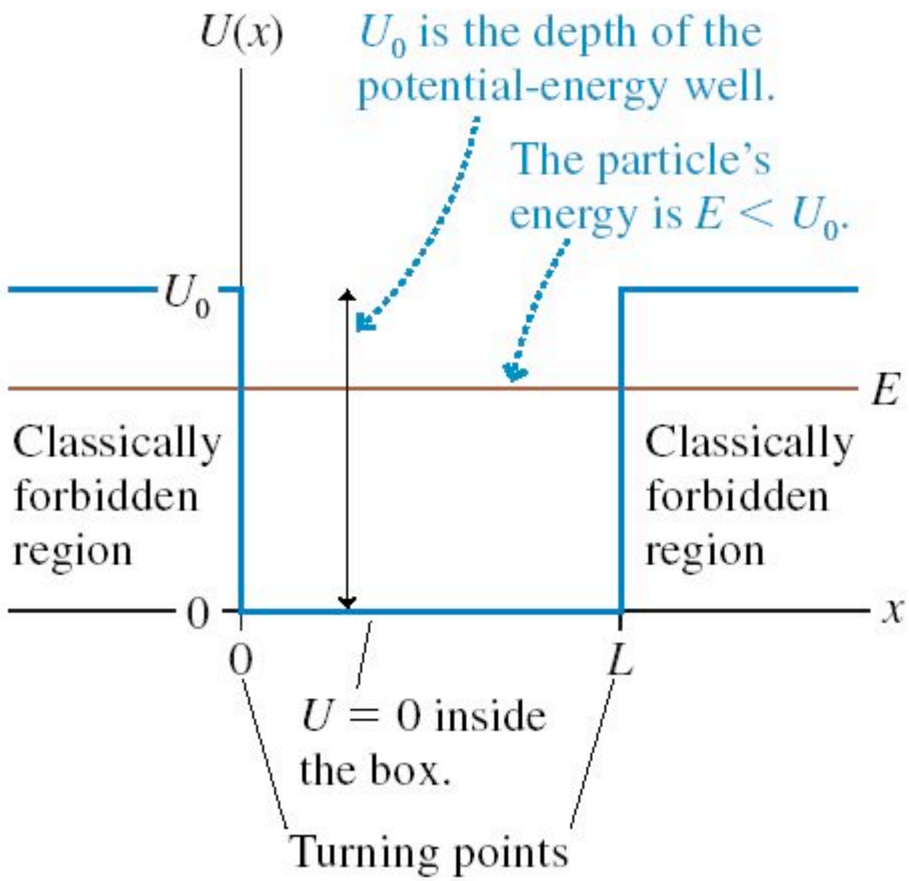
The wave function oscillates until it reaches the classical turning point at $x = L$, then it decays exponentially within the classically forbidden region. A similar analysis can be done for $x \leq 0$.

We can define a parameter _ defined as the distance into the classically forbidden region at which the wave function has decreased to e^{-1} or 0.37 times its value at the edge:

$$\text{penetration distance } \eta = \frac{\hbar}{\sqrt{2m(U_0 - E)}}$$

FIGURE 41.13 A finite potential well of width L and depth U_0.

(a) $U = 0$ inside the well.



$$\frac{\partial^2}{\partial x^2}\hat{\psi}(x) = -\beta^2(x)\hat{\psi}(x)$$

$$\beta^2(x) = \frac{2m}{\hbar^2}\left(E - U(x)\right)$$

Outside $\quad \beta^2(x) < 0$

$$\frac{\partial^2}{\partial x^2}\hat{\psi}(x) = \frac{1}{\eta^2}\hat{\psi}(x)$$

$$\frac{1}{\eta^2} = \frac{2m}{\hbar^2}\left(U_0 - E\right)$$

Solution, x>L

$$\hat{\psi}(x) = \hat{\psi}_{edge}\exp[-(x-L)/\eta]$$

The Quantum Harmonic Oscillator

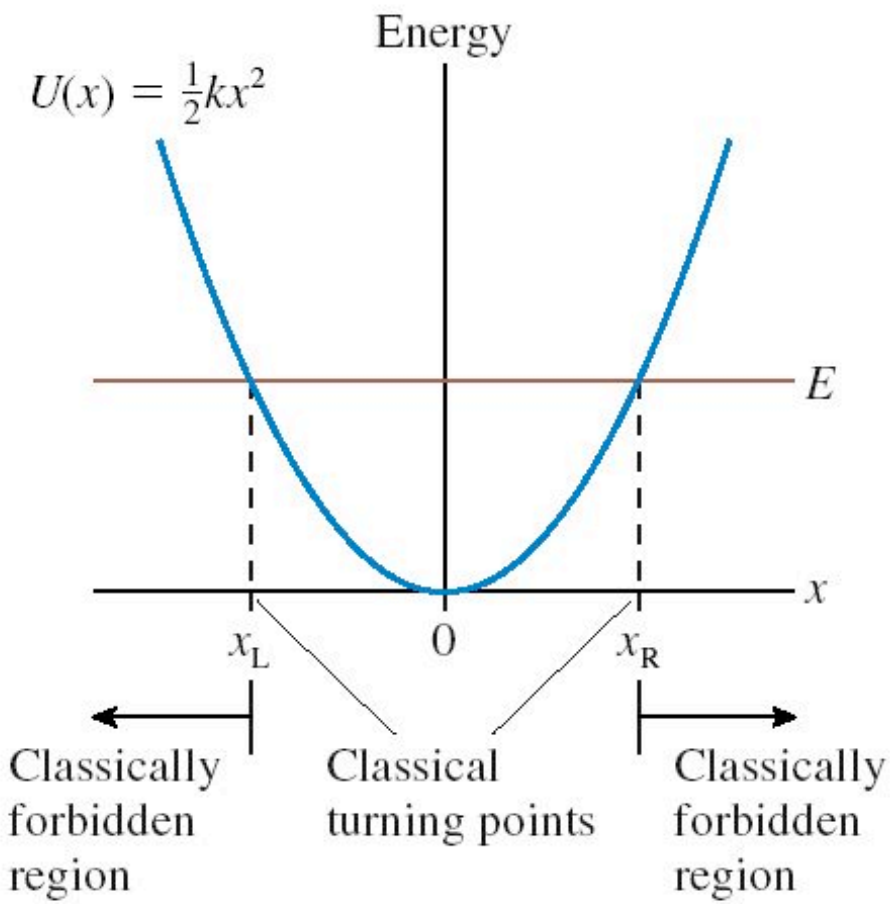
The potential-energy function of a harmonic oscillator, as you learned in Chapter 10, is

$$U(x) = \frac{1}{2}kx^2$$

where we'll assume the equilibrium position is $x_e = 0$. The Schrödinger equation for a quantum harmonic oscillator is then

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}\left(E - \frac{1}{2}kx^2\right)\psi(x)$$

FIGURE 41.20 The potential energy of a harmonic oscillator.



The Quantum Harmonic Oscillator

The wave functions of the first three states are

$$\psi_1(x) = A_1 e^{-x^2/2b^2}$$

$$\psi_2(x) = A_2 \frac{x}{b} e^{-x^2/2b^2}$$

$$\psi_3(x) = A_3\left(1 - \frac{2x^2}{b^2}\right)e^{-x^2/2b^2}$$

$$b = \sqrt{\frac{\hbar}{m\omega}}$$

$$E_n = \left(n - \frac{1}{2}\right)\hbar\omega \qquad n = 1, 2, 3, \ldots$$

Where $\omega = (k/m)^{1/2}$ is the classical angular frequency, and n is the quantum number

FIGURE 41.21 The first three energy levels and wave functions of a quantum harmonic oscillator.

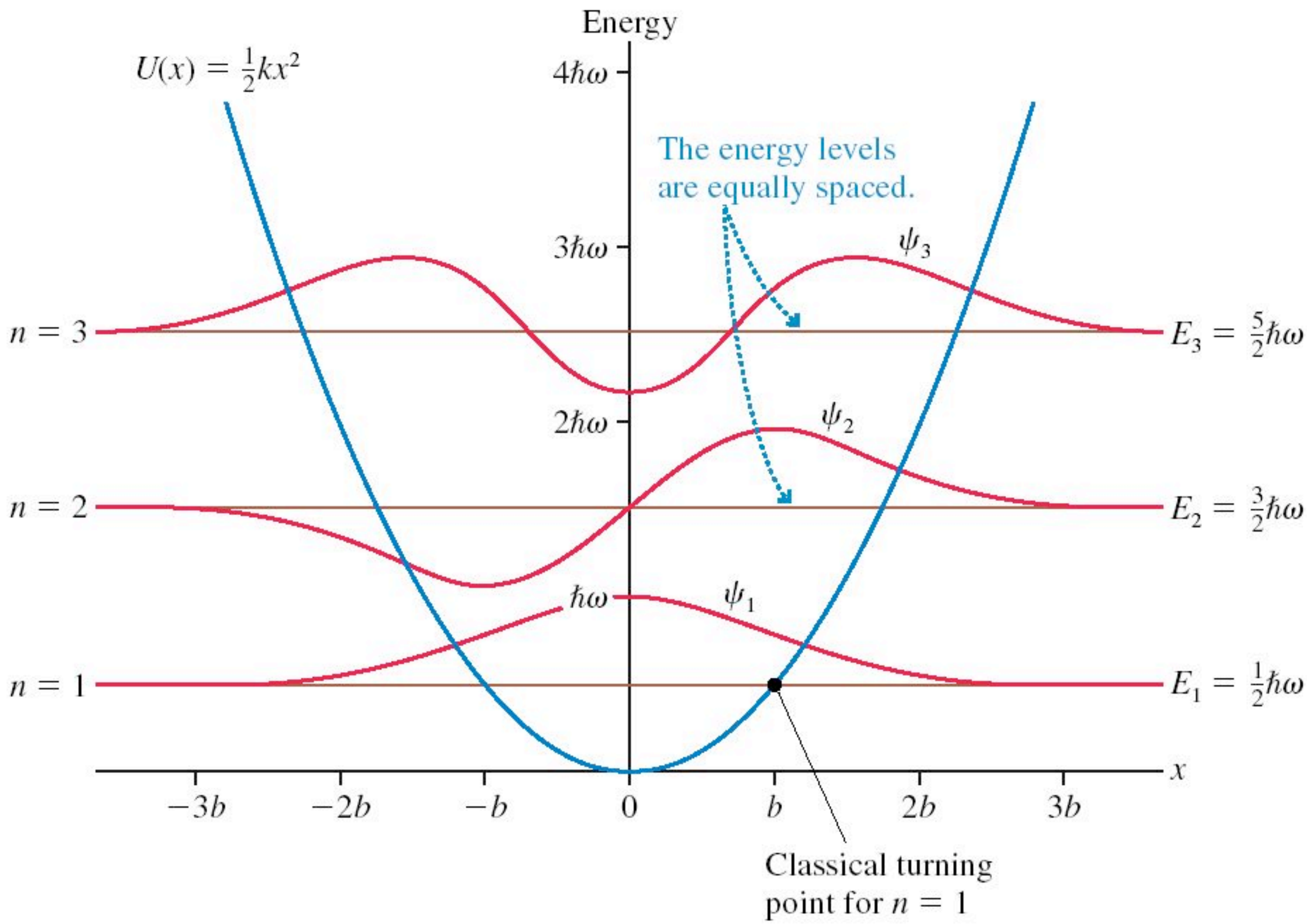
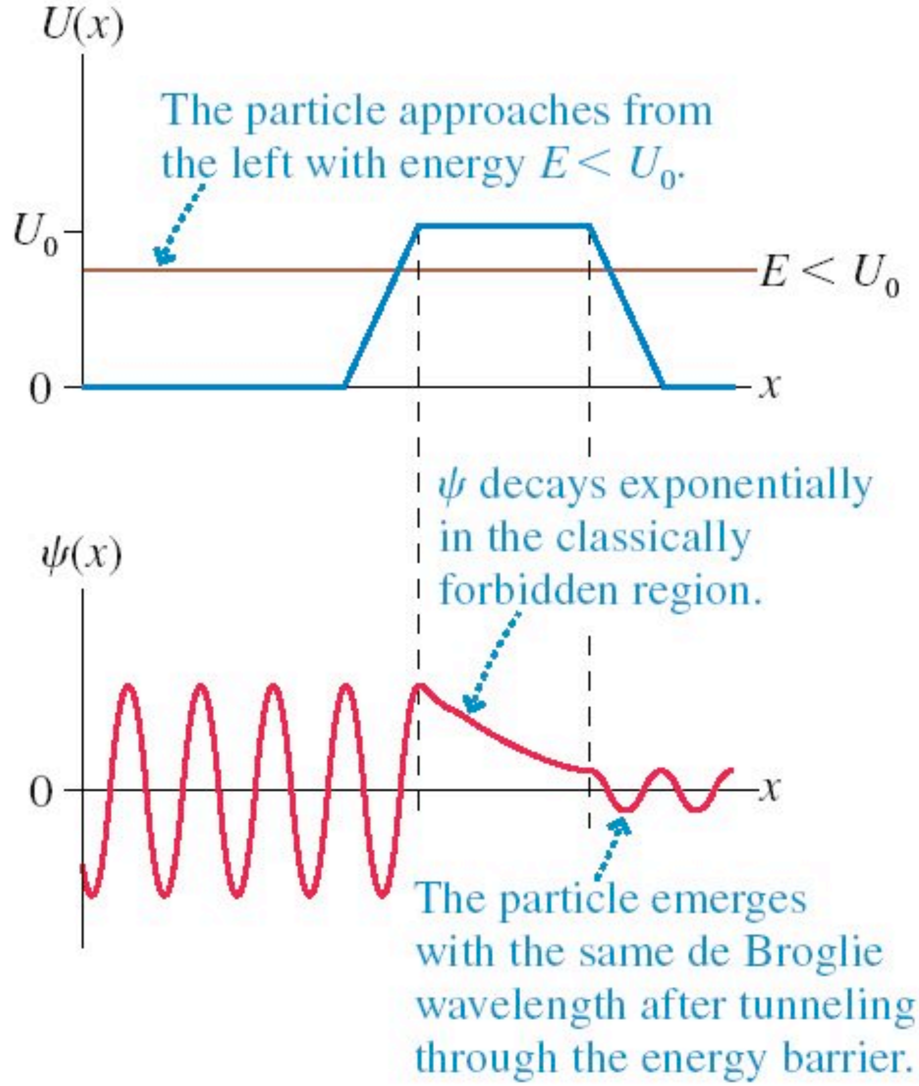


FIGURE 41.30 A quantum particle can penetrate through the energy barrier.



Quantum-Mechanical Tunneling

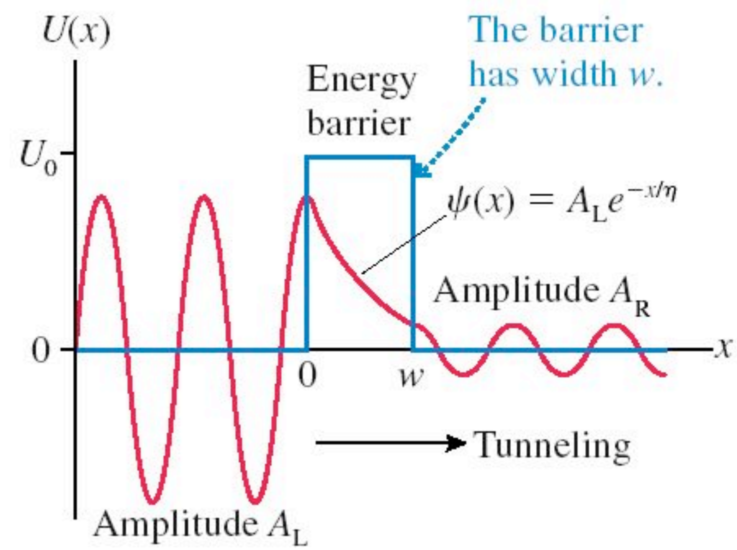
Once the penetration distance η is calculated using

$$\frac{1}{\eta^2} = \frac{2m}{\hbar^2}(U_0 - E)$$

probability that a particle striking the barrier from the left will emerge on the right is found to be

$$P_{\text{tunnel}} = \frac{|A_R|^2}{|A_L|^2} = (e^{-w/\eta})^2 = e^{-2w/\eta}$$

FIGURE 41.31 Tunneling through an idealized energy barrier.



THE END !

Good Luck on the remaining exams