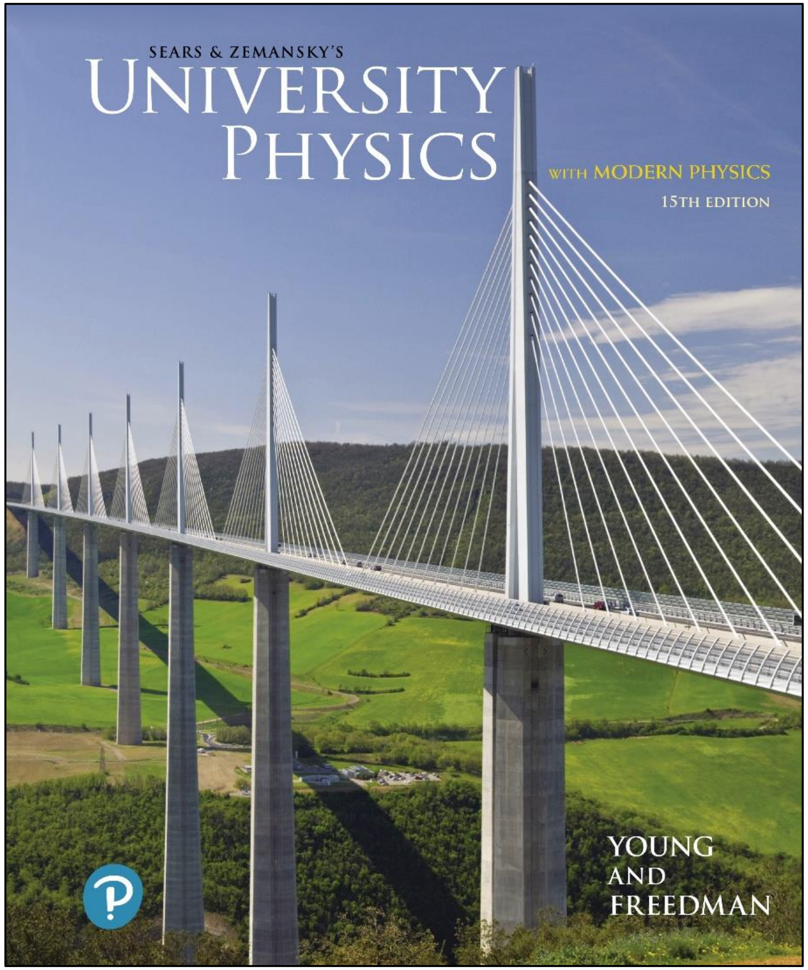
University Physics with Modern Physics

Fifteenth Edition



Chapter 40

Quantum Mechanics I: Wave Functions

Pearson

Learning Outcomes

In this chapter, you'll learn…

- the wave function that describes the behavior of a particle and the **Schrödinger equation** that this function must satisfy.
- how to calculate the wave functions and energy levels for a particle confined to a box, and for a harmonic oscillator.
- how quantum mechanics makes it possible for particles to go where Newtonian mechanics says they cannot: **quantum tunneling**.
- how **measuring** a quantum-mechanical system can change that system's state.

Introduction

- Just as we use the wave equation to analyze waves on a string or sound waves in a pipe, we can use a related equation—the **Schrödinger equation**—to analyze the behavior of matter from a quantum-mechanical perspective.
- In the photograph, microscopic particles of different sizes fluoresce under ultraviolet light.
- The smaller the particles, the shorter the wavelength of visible light they emit.
- The Schrödinger equation will help us understand why.

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The Schrödinger Equation in 1-D (1 of 2)

- In a one-dimensional model, a quantum-mechanical particle is described by a wave function $\Psi(x,t)$.
- The one-dimensional Schrödinger equation for a free particle of mass *m* is:

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

- The presence of *i* (the square root of –1) in the Schrödinger equation means that wave functions are always complex functions.
- The square of the absolute value of the wave function, $|\Psi(x,t)|^2$, is called the probability distribution function. It tells us about the probability of finding the particle near position *x* at time *t*.
- Video Tutor Solution: Example 40.1

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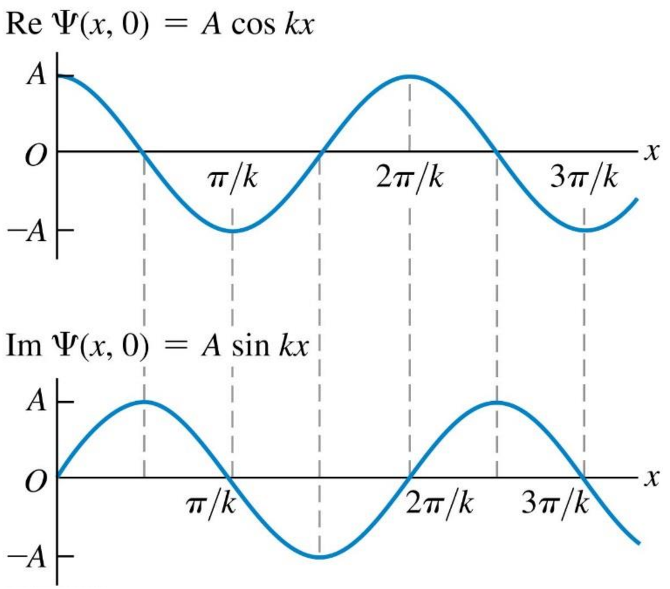
The Schrödinger Equation in 1-D: A Free Particle

- A free particle can have a definite momentum $p = \hbar k$ and energy $E = \hbar\omega$.
- Such a particle is not localized at all: The wave function extends to infinity.
- The wave function can be written as a complex exponential:



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

(sinusoidal wave function representing a new particle)

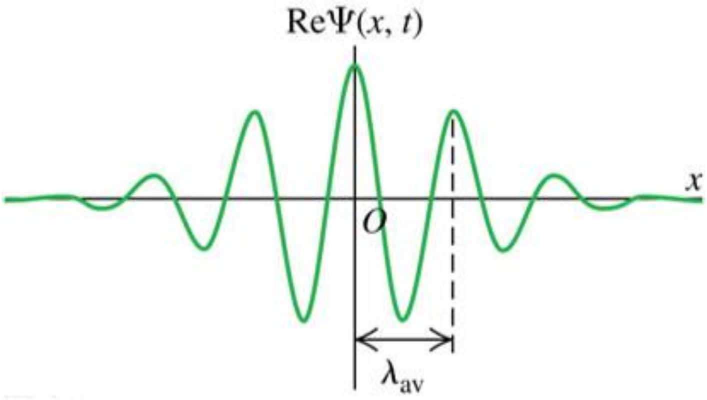
The Schrödinger Equation in 1-D: Wave Packets (1 of 2)

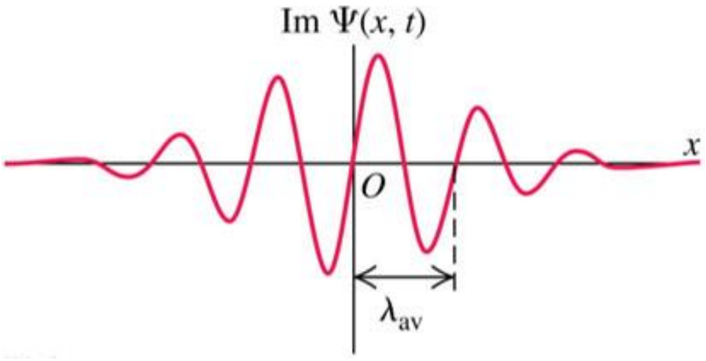
- Superposing a large number of sinusoidal waves with different wave numbers and appropriate amplitudes can produce a wave pulse that has a wavelength

$$\lambda_{av} = \frac{2\pi}{k_{av}}$$

  and is localized within a region of space of length Δx.

- Shown are the real and imaginary components of such a wave packet at time t.





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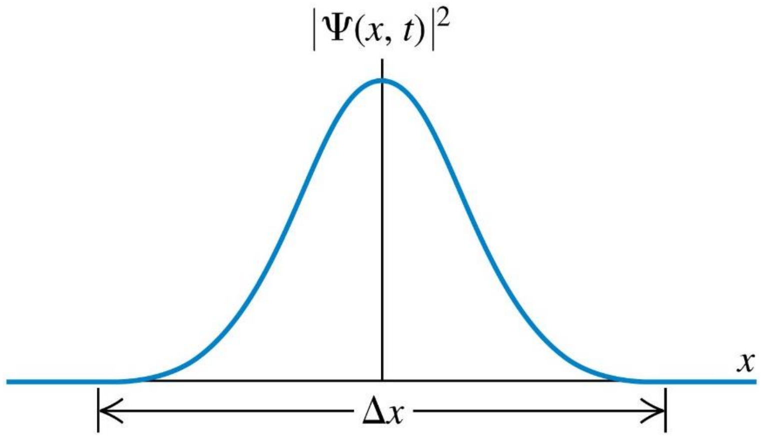
The Schrödinger Equation in 1-D: Wave Packets (2 of 2)

- The resulting probability distribution has only one maximum.
- This localized pulse has aspects of both particle and wave.
- It is a particle in the sense that it is localized in space; if we look from a distance, it may look like a point.
- But it also has a periodic structure that is characteristic of a wave.
- Such a localized wave pulse is called a **wave packet**.



The Schrödinger Equation in 1-D (2 of 2)

- If a particle of mass *m* moves in the presence of a potential energy function *U*(*x*), the one-dimensional Schrödinger equation for the particle is:

General one-dimensional Schrödinger equation:

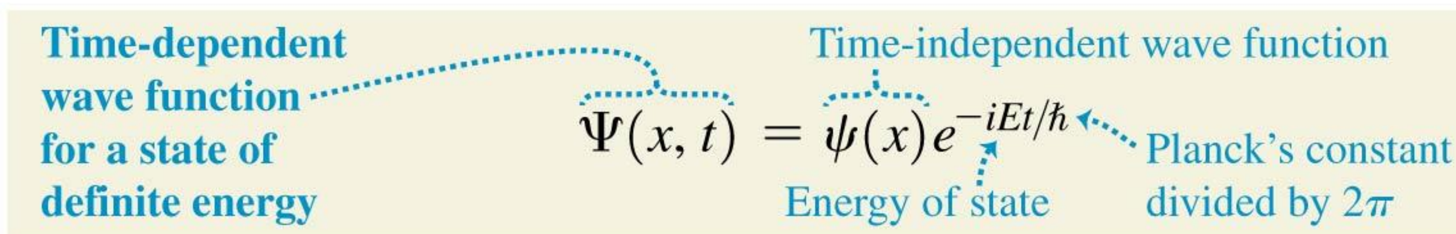
$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

Planck's constant divided by 2π ($\hbar$); Particle's wave function ($\Psi(x,t)$); Particle's mass (m); Potential-energy function ($U(x)$)

- Note that if *U*(*x*) = 0, this reduces to the free-particle Schrödinger equation.

The Schrödinger Equation in 1-D: Stationary States (1 of 2)

- If a particle has a definite energy *E*, the wave function $\Psi(x,t)$ is a product of a time-independent wave function $\Psi(x)$ and a factor that depends on time *t* but not position:



- For such a **stationary state** the probability distribution function $\left|\Psi(x,t)\right|^2 = \left|\Psi(x)\right|^2$ does not depend on time.

The Schrödinger Equation in 1-D: Stationary States (2 of 2)

- The time-independent one-dimensional Schrödinger equation for a stationary state of energy *E* is:

Time-independent one-dimensional Schrödinger equation:

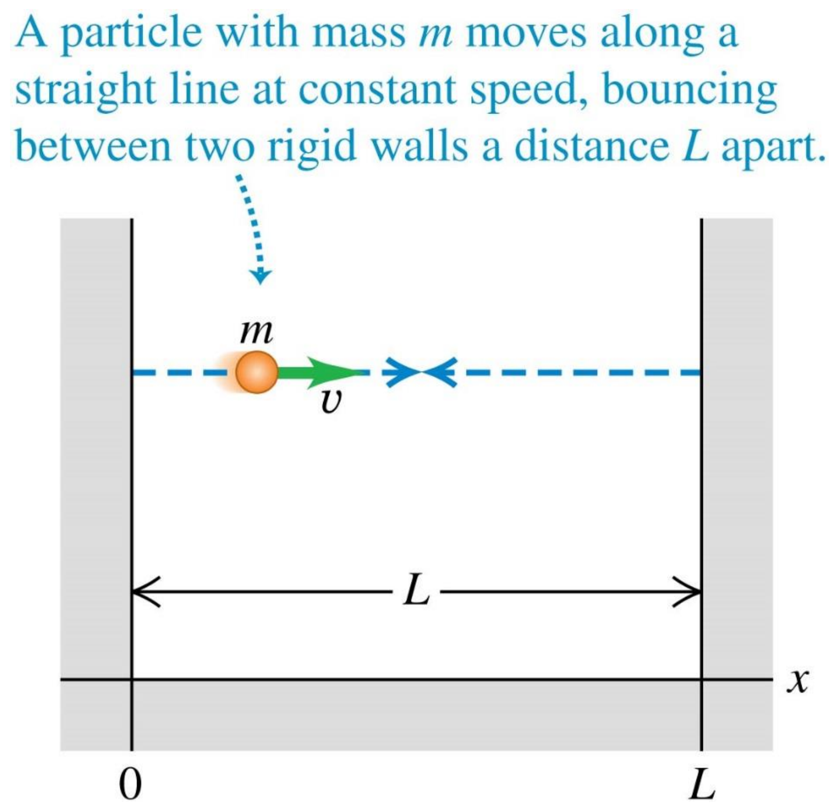
$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x)$$

Planck's constant divided by 2π ($\hbar$); Time-independent wave function ($\psi(x)$); Particle's mass (m); Potential-energy function ($U(x)$); Energy of state (E)

- Much of Chapter 40 is devoted to solving this equation to find the definite-energy, stationary-state wave functions $\Psi(x)$ and the corresponding values of *E*—that is, the energies of the allowed levels—for different physical situations.
- Video Tutor Solution: Example 40.2

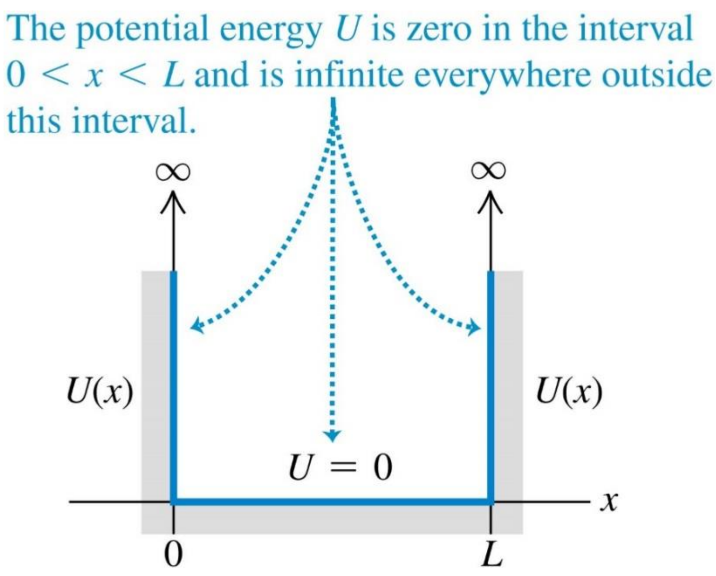
Newtonian View of a Particle in a Box

- Let's look at a simple model in which a particle is bound so that it cannot escape to infinity, but rather is confined to a restricted region of space.
- Our system consists of a particle confined between two rigid walls separated by a distance *L*.



Potential Energy for a Particle in a Box

- The potential energy corresponding to the rigid walls is infinite, so the particle cannot escape.
- This model might represent an electron that is free to move within a long, straight molecule or along a very thin wire.



Particle in a Box: Wave Functions, Energy Levels (1 of 2)

- The energy levels for a particle in a box are:

Energy levels for a particle in a box; Magnitude of momentum; Planck's constant; Planck's constant divided by 2π

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

Particle's mass; Width of box; Quantum number

- Each energy level has its own value of the quantum number *n* and a corresponding wave function:

Stationary-state wave functions for a particle in a box; Quantum number

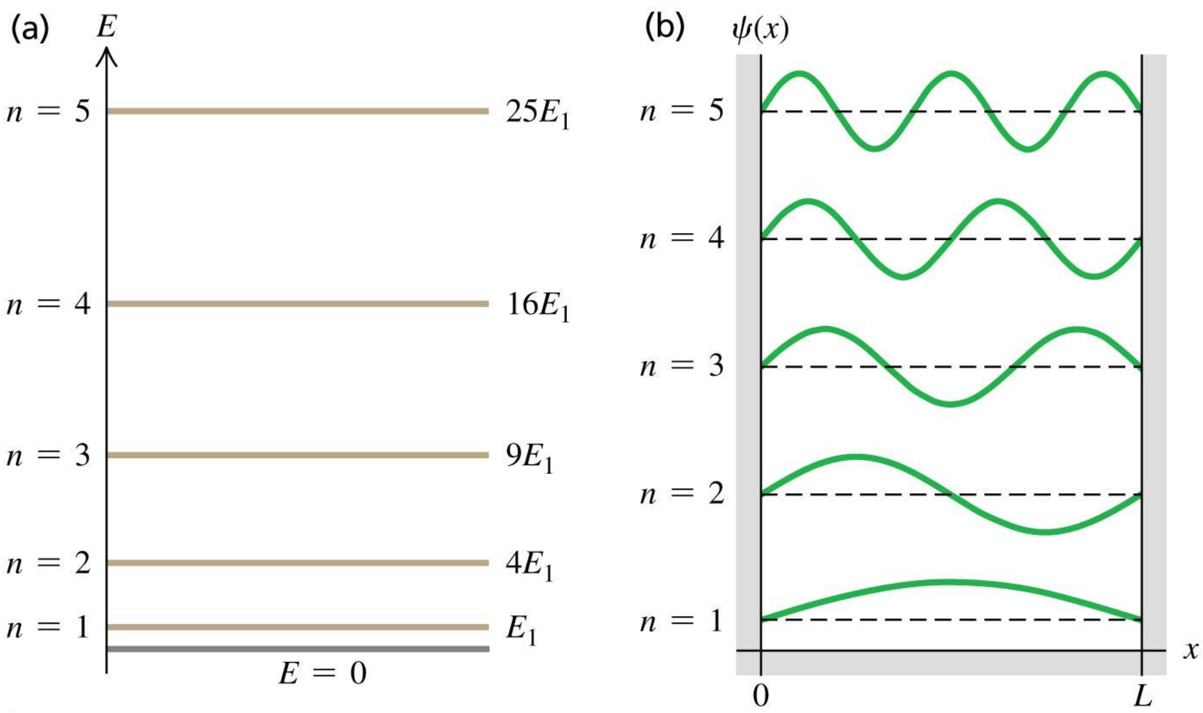
$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad (n = 1, 2, 3, \ldots)$$

Width of box

- Video Tutor Solution: Example 40.6

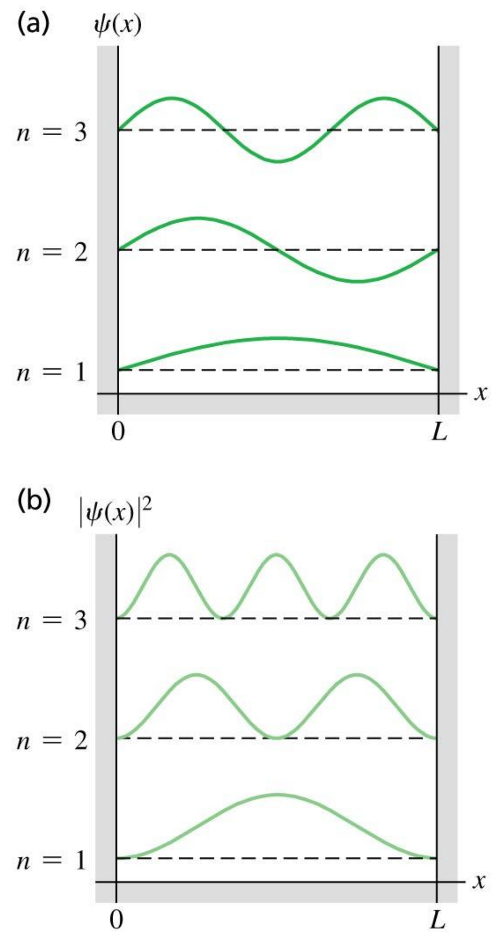
Particle in a Box: Wave Functions, Energy Levels (2 of 2)

- Shown are energy levels and associated stationary-state wave functions for a particle in a box.



Particle in a Box: Probability and Normalization

- Shown are the first three $\Psi(x)$ stationary-state wave functions for a particle in a box (a) and the associated the associated probability distribution functions $|\Psi(x)|^2$ (b).
- There are locations where there is **zero** probability of finding the particle.
- Wave functions must be normalized so that the integral of $|\Psi(x)|^2$ over all x equals 1 (means there is 100% probability of finding the particle **somewhere**).



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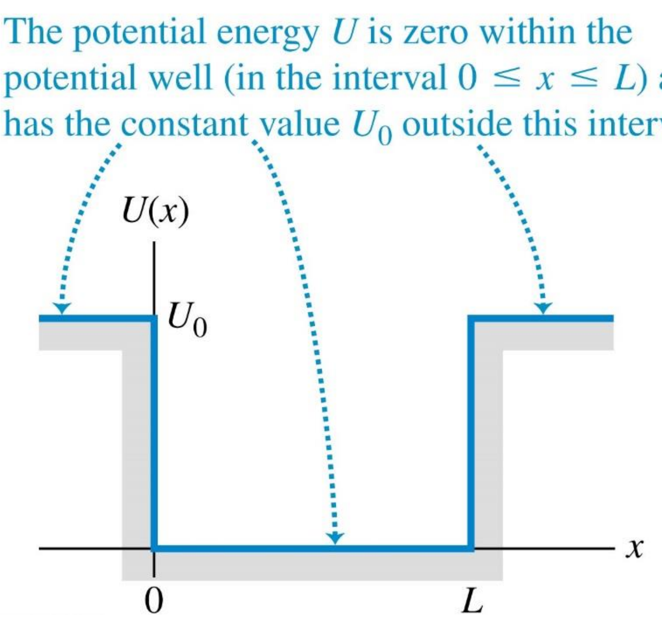
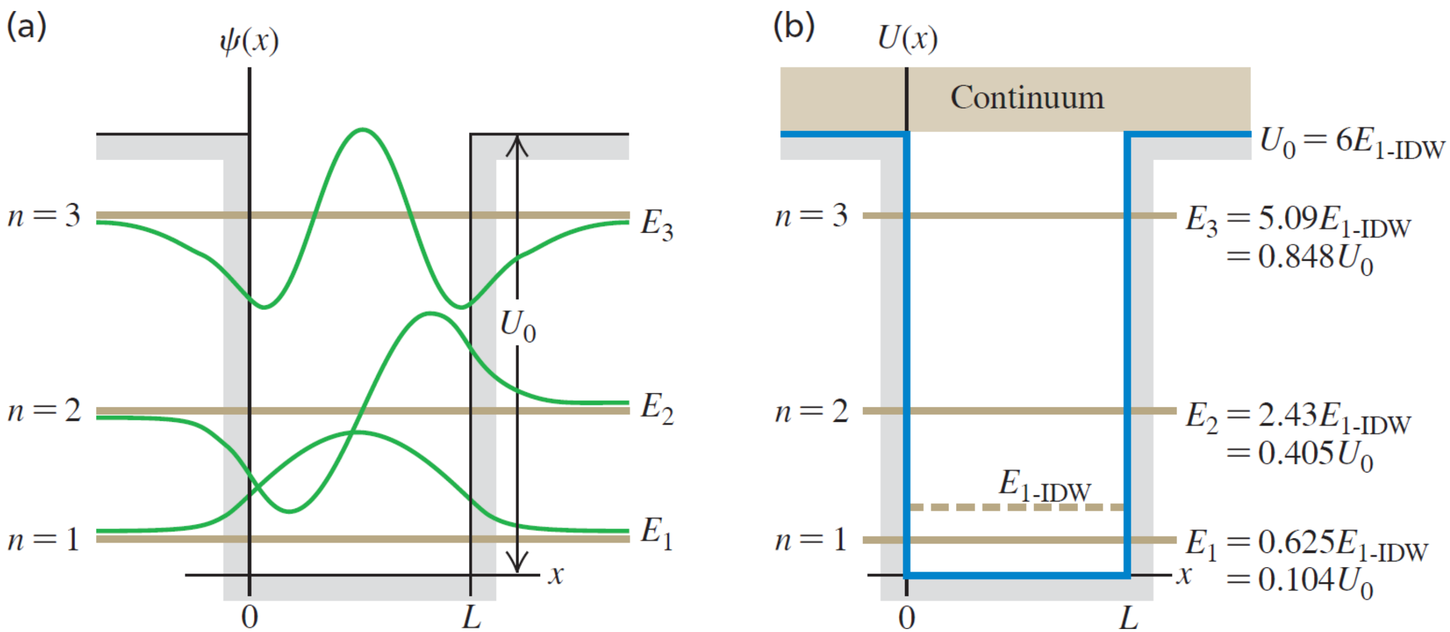
Particle in a Finite Potential Well (1 of 3)

- A **finite well** is a potential well that has straight sides but finite height.
- This function is often called a **square-well potential**.



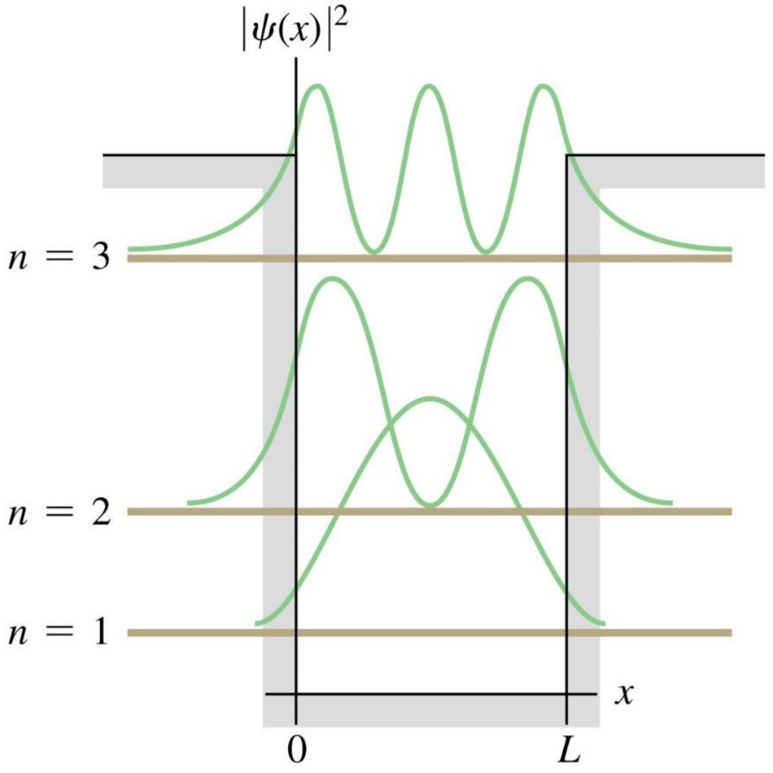
Particle in a Finite Potential Well (2 of 3)

- Shown are the stationary-state wave functions $\Psi(x)$ and corresponding energies for one particular finite well.
- All energies greater than U_0 are possible; states with $E > U_0$ form a continuum.



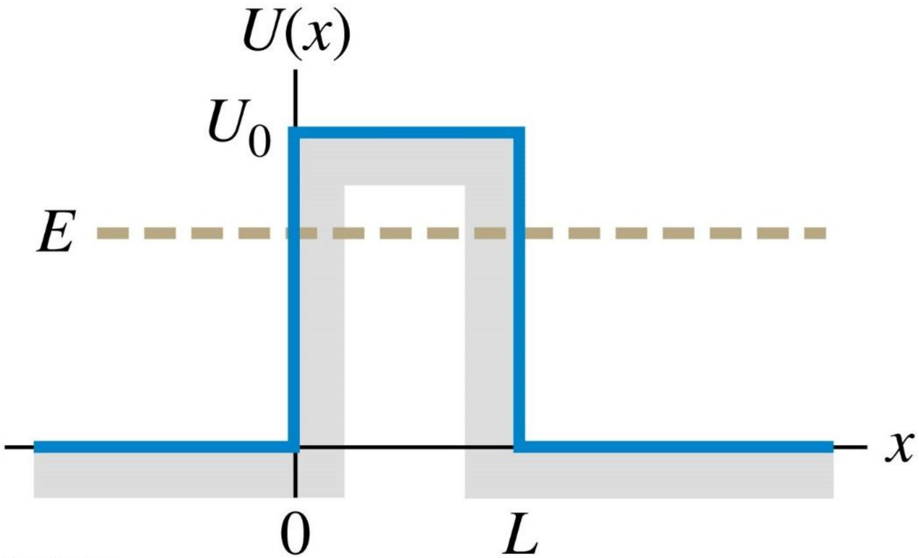
Particle in a Finite Potential Well (3 of 3)

- Shown are graphs of the probability distributions for the first three bound states of a finite well.
- As with the infinite well, not all positions are equally likely.
- Unlike the infinite well, there is some probability of finding the particle outside the well in the classically forbidden regions.



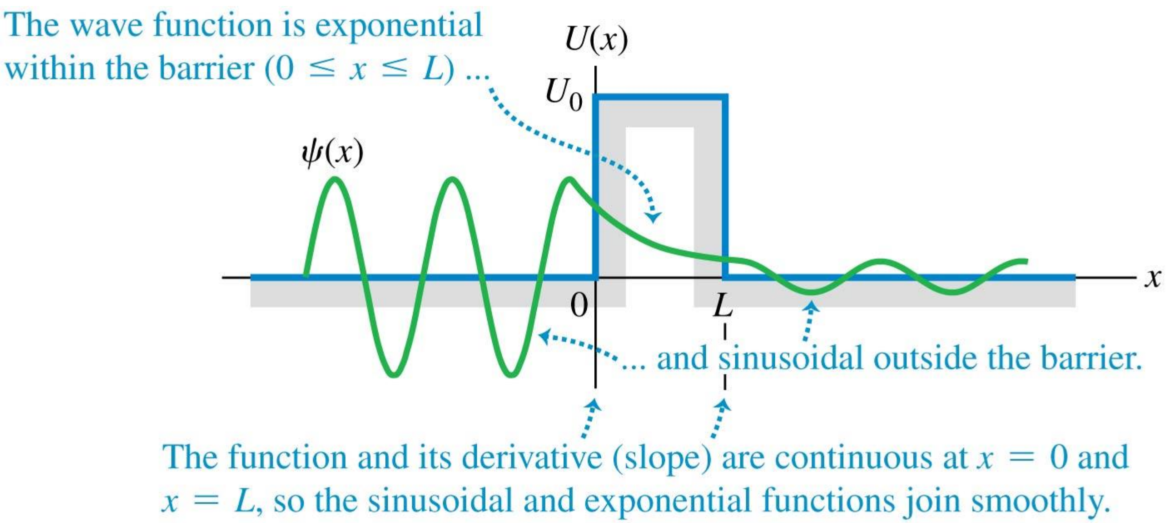
Potential Barriers and Tunneling (1 of 2)

- Shown below is a potential barrier.
- In Newtonian physics, a particle whose energy E is less than the barrier height U_0 cannot pass from the left-hand side of the barrier to the right-hand side.



Potential Barriers and Tunneling (2 of 2)

- Shown below is the wave function $\Psi(x)$ for a free particle that encounters a potential barrier.
- The wave function is nonzero to the right of the barrier, so it is possible for the particle to "tunnel" from the left-hand side to the right-hand side.



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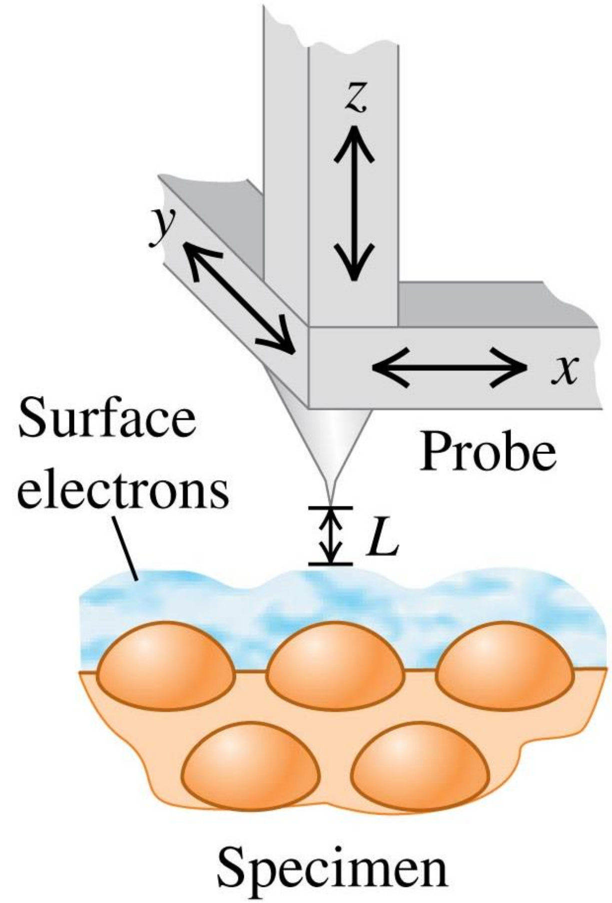
Scanning Tunneling Microscope (STM) (1 of 2)

- The scanning tunneling microscope (STM) uses electron tunneling to create images of surfaces down to the scale of individual atoms.
- An extremely sharp conducting needle is brought very close to the surface, within 1 nm or so.
- When the needle is at a positive potential with respect to the surface, electrons can tunnel through the surface potential-energy barrier and reach the needle.



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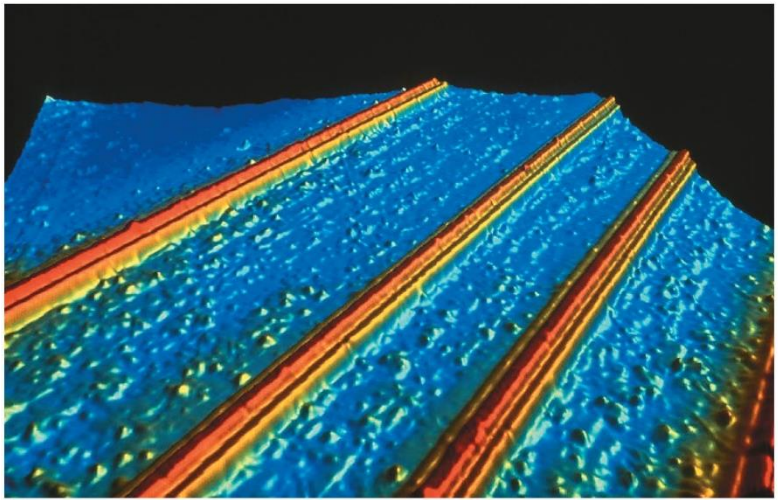
Scanning Tunneling Microscope (STM) (2 of 2)

- This colored STM image shows “quantum wires:” thin strips, just 10 atoms wide, of a conductive rare-earth silicide atop a silicon surface.
- Such quantum wires may one day be the basis of ultraminiaturized circuits.



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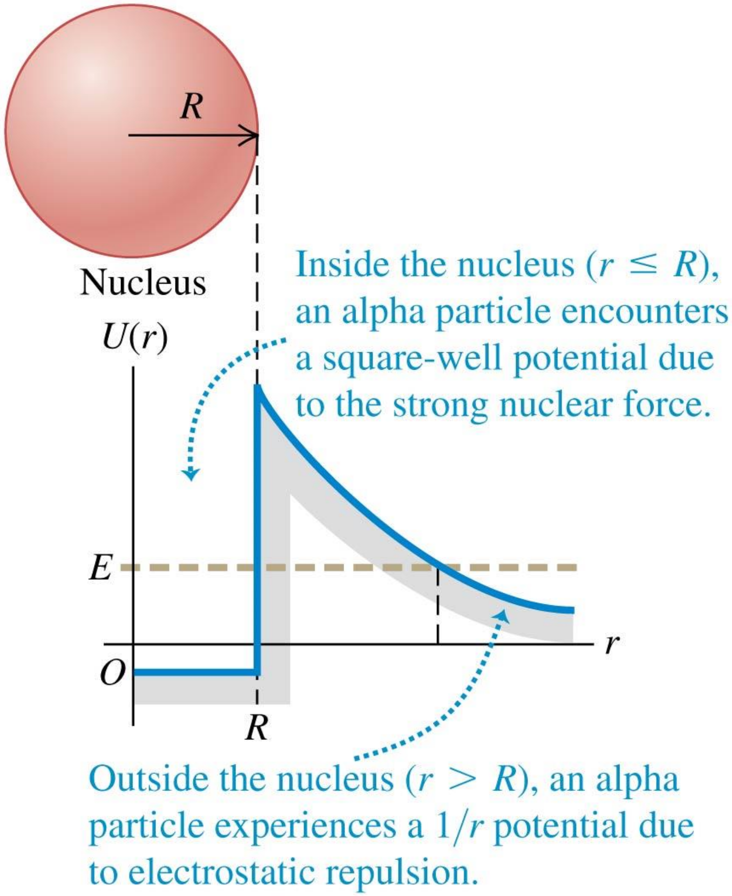
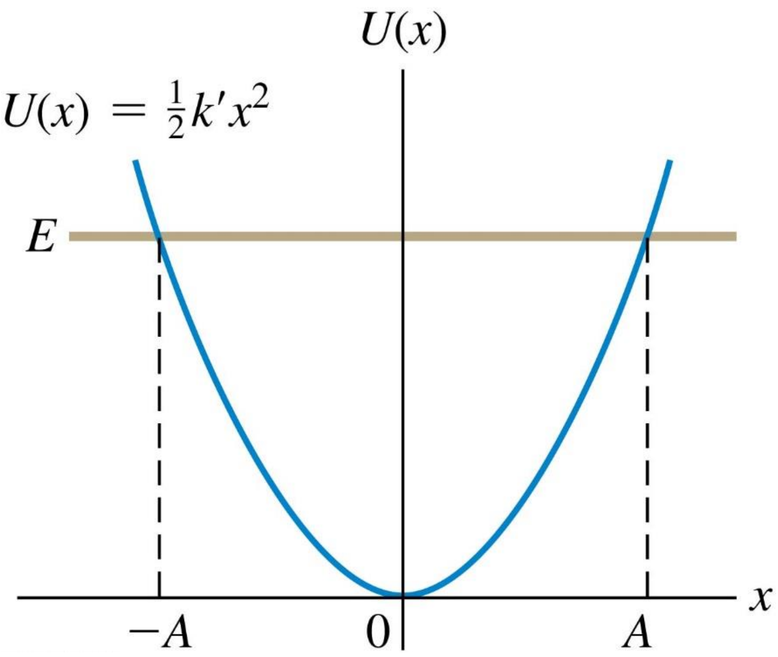
Applications of Tunneling

- Tunneling is of great importance in nuclear physics.
- An alpha particle trying to escape from a nucleus encounters a potential barrier that results from the combined effect of the attractive nuclear force and the electrical repulsion of the remaining part of the nucleus.
- To escape, the alpha particle must tunnel through this barrier.



The Harmonic Oscillator (1 of 2)

- Shown is the potential-energy function for the harmonic oscillator.
- In Newtonian mechanics the particle is restricted to the range from $x = -A$ to $x = A$.
- In quantum mechanics the particle can be found at $x > A$ or $x < -A$.



Energy Levels for a Harmonic Oscillator

- The allowed energies for a harmonic oscillator are:

Energy levels for a harmonic oscillator

$$E_n = \left(n + \tfrac{1}{2}\right)\hbar\sqrt{\frac{k'}{m}} = \left(n + \tfrac{1}{2}\right)\hbar\omega \quad (n = 0, 1, 2, \ldots)$$

Quantum number; Planck's constant divided by 2π; Particle's mass; Force constant; Oscillation angular frequency

- Note that the ground level of energy E_0 is denoted by the quantum number $n = 0$, not $n = 1$.
- There are infinitely many levels.
- As $|x|$ increases, $U = \tfrac{1}{2}k'x^2$ increases without bound.

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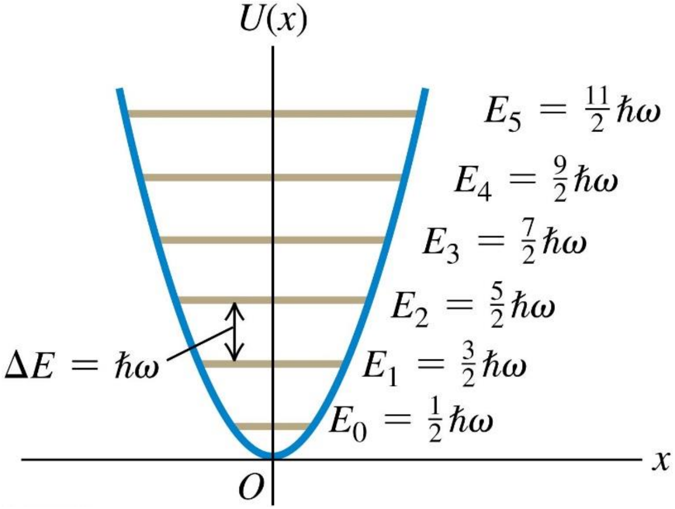
The Harmonic Oscillator (2 of 2)

- Shown are the lowest six energy levels of the harmonic oscillator, and the potential-energy function $U(x)$.
- For each level n, the value of $|x|$ at which the horizontal line representing the total energy E_n intersects $U(x)$ gives the amplitude A_n of the corresponding Newtonian oscillator.



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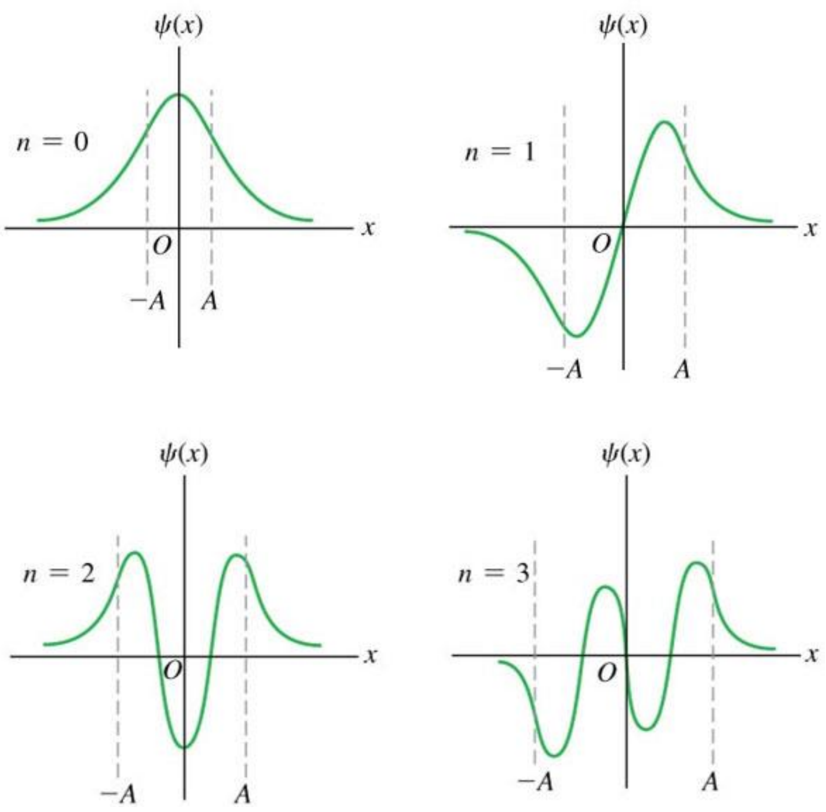
Wave Functions for the Harmonic Oscillator

- Shown are the first four stationary-state wave functions $\Psi(x)$ for the harmonic oscillator.
- *A* is the amplitude of oscillation in Newtonian physics.



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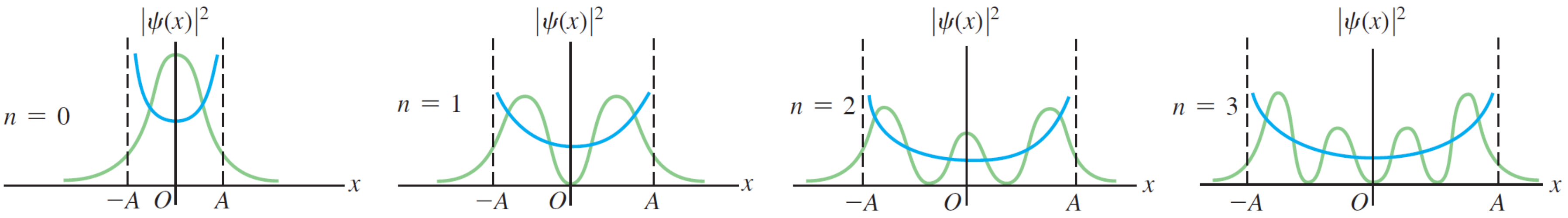
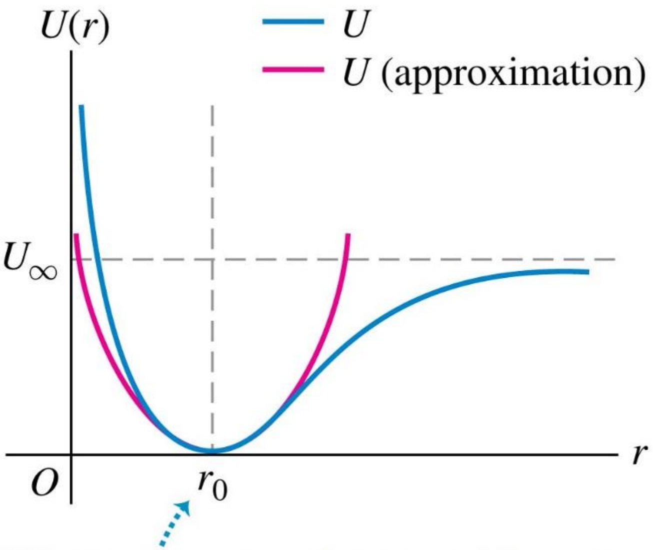
Probability Distributions for the Harmonic Oscillator

- Shown are the probability distribution functions for the first four stationary-state wave functions for the harmonic oscillator.
- The blue curves are the Newtonian probability distributions.



Modeling a Diatomic Atom

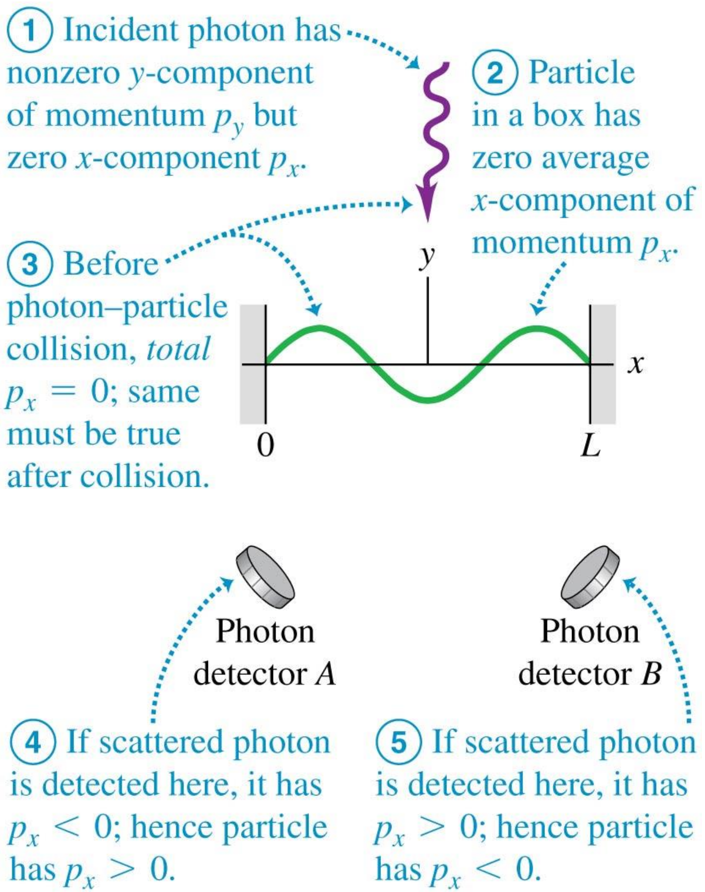
- A potential-energy function describing the interaction of two atoms in a diatomic molecule.
- The distance *r* is the separation between the centers of the atoms.



When r is near r_0, the potential-energy curve is approximately parabolic (as shown by the red curve) and the system behaves approximately like a harmonic oscillator.

Measurement in Quantum Mechanics

- Shown is a method for using photon scattering to measure the *x*-component of momentum of a particle in a box.
- Even when we use a photon with the lowest possible momentum, we find that the state of the particle in the box must **change** as a result of the experiment.



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