PHY1203: General Physics III

Chapter 40
Quantum Mechanics – Part 2

Particle in a box: Time dependence

- The wave functions ψ_n(x) depend only on the spatial coordinate x.
- We know that the full time-dependent wave function is

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

- Therefore the time-dependent stationary-state wave functions for a particle in a box are

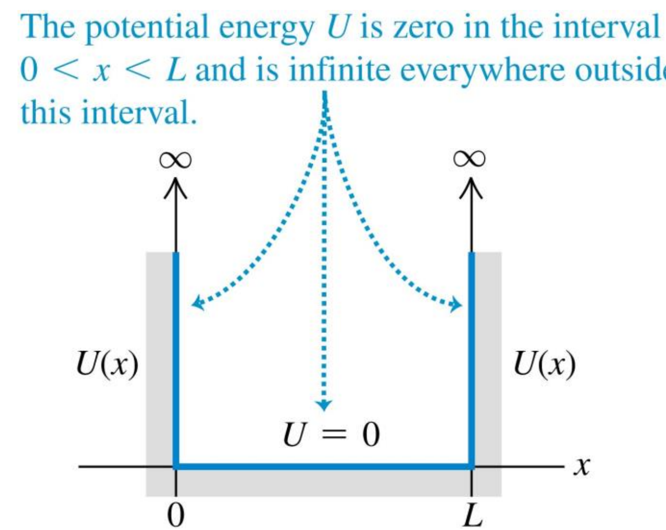
$$\Psi_n(x,t) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)e^{-iE_n t/\hbar} \qquad (n = 1, 2, 3, \ldots)$$

- The energy E_n is as before. The higher the quantum number *n* is, the faster it oscillates.
- The probably distribution function $|\Psi_n(x,t)|^2 = (2/L)\sin^2(n\pi x/L)$ is independent of time (stationary!)

Particle in a box: Review

- The Schrödinger equation in the potential well:

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



- Outside the potential well: $\psi(x)=0$
- Solution: $\psi(x) = A_1 e^{ikx} + A_2 e^{-ikx}$

Stationary-state wave functions for a particle in a box

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

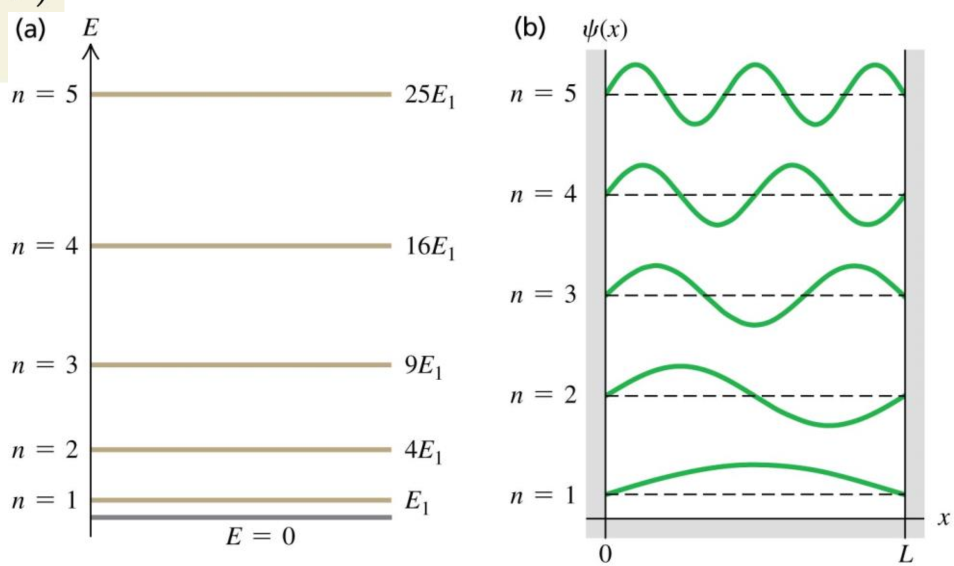
Quantum number

Width of box

Energy levels for a particle in a box

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

Magnitude of momentum; Planck's constant; Planck's constant divided by 2π; Particle's mass; Width of box; Quantum number

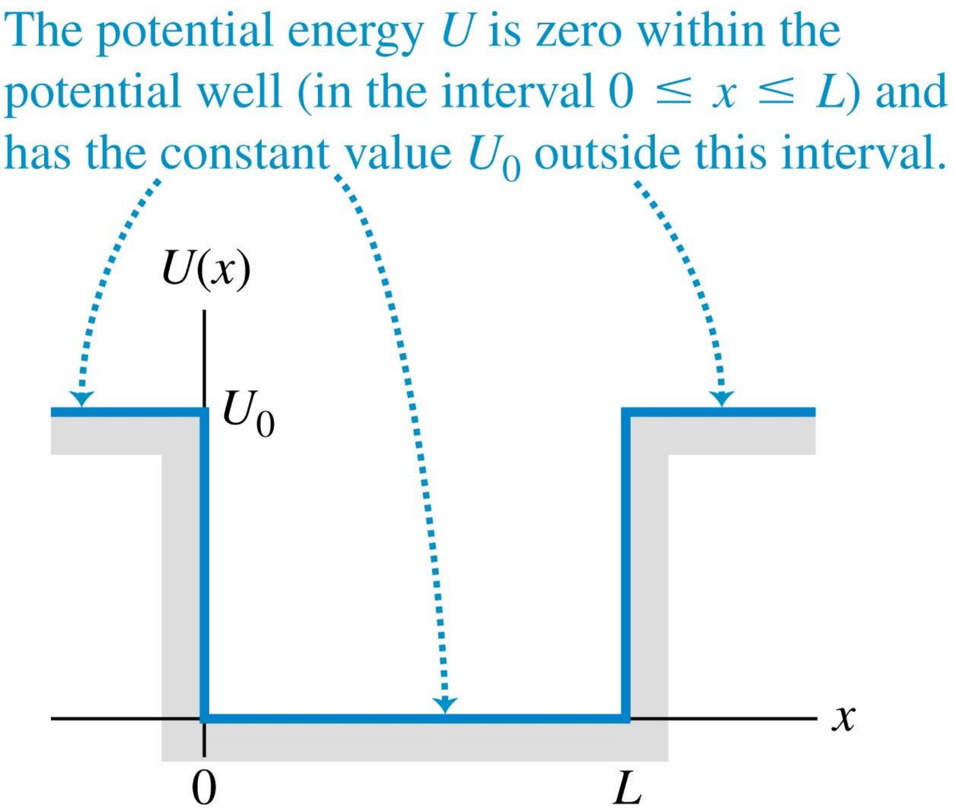


with time dependence:

$$\Psi_n(x,t) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)e^{-iE_n t/\hbar} \qquad (n = 1, 2, 3, \ldots)$$

Particle in a finite potential well

- A **finite well** is a potential well that has straight sides but finite height.
- This function is often called a **square-well potential**.
- Newtonian view: the particle is trapped (localized) in a well if the total mechanical energy E is less than U_0.
- In quantum mechanics, such a trapped state is often called a bound state. All states are bound for an infinitely deep well.



- In Newtonian view, if E is greater than U_0, the particle is not bound.

Particle in a finite potential well

- Let us solve the the Schrödinger equation. For [0, L] we have

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

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

- which looks the same as that of the infinite potential well. The difference is for x outside [0, L]: the potential energy is no longer infinity, and the wave function is no longer zero. For $x < 0$ or $x > L$, the Schrödinger equation looks like

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

- Since U_0-E is positive, the solution must be exponential. The solution can be written as

$$\psi(x) = Ce^{\kappa x} + De^{-\kappa x} \qquad \text{(outside the well)}$$

- For $x < 0$, D must be 0; For $x > L$, C must be 0. (ψ cannot be infinity as $x \rightarrow \pm\infty$)

Particle in a finite potential well

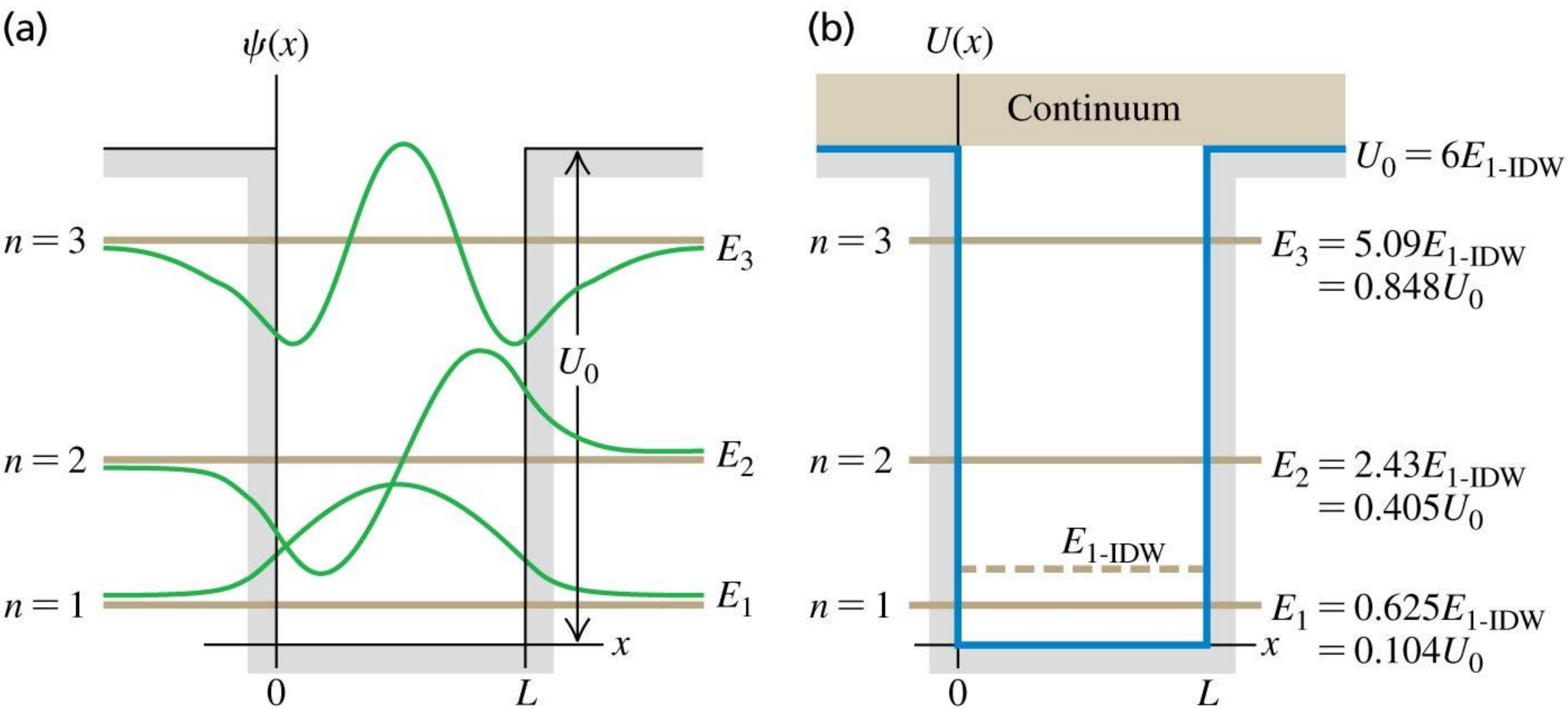
- We need to *match* the boundary condition that $\psi(x)$ and $d\psi(x)/dx$ must be continuous at the boundary points $x = 0$ and L.

- If the wave function $\psi(x)$ or the slope $d\psi(x)/dx$ were to change discontinuously at a point, the second derivative $d^2\psi(x)/dx^2$ would be *infinite* at that point, which violate the the Schrödinger equation which says that at *every point* $d^2\psi(x)/dx^2$ is proportional to $U - E$.

- Matching the sinusoidal and exponential functions at the boundary points, in most cases, requires numerical solution.

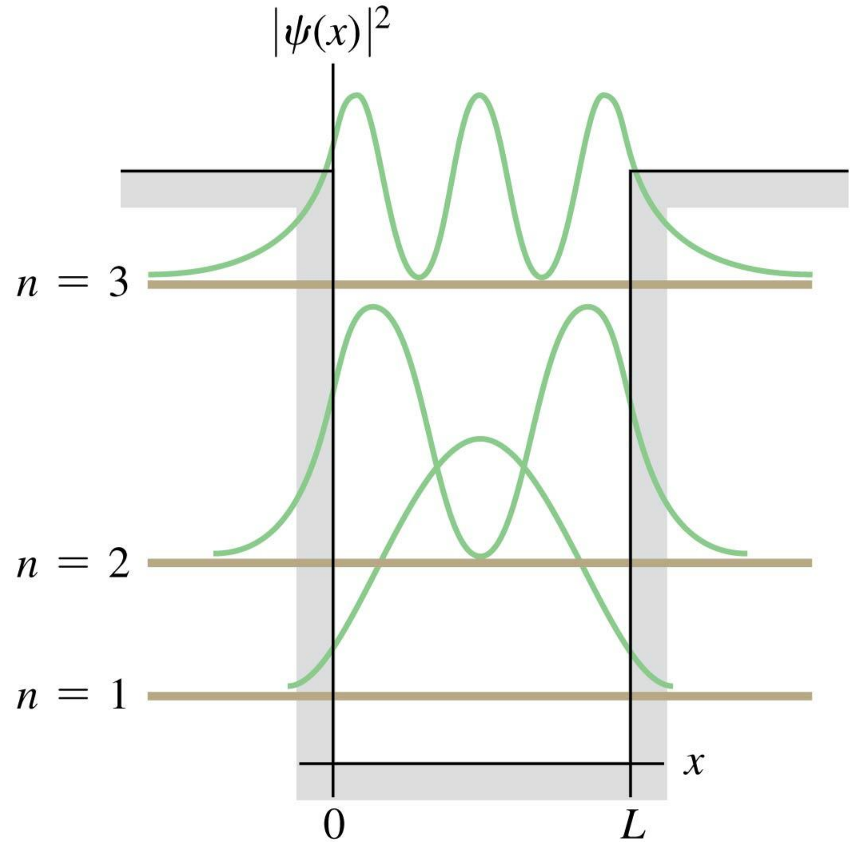
Particle in a finite potential well

- 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.



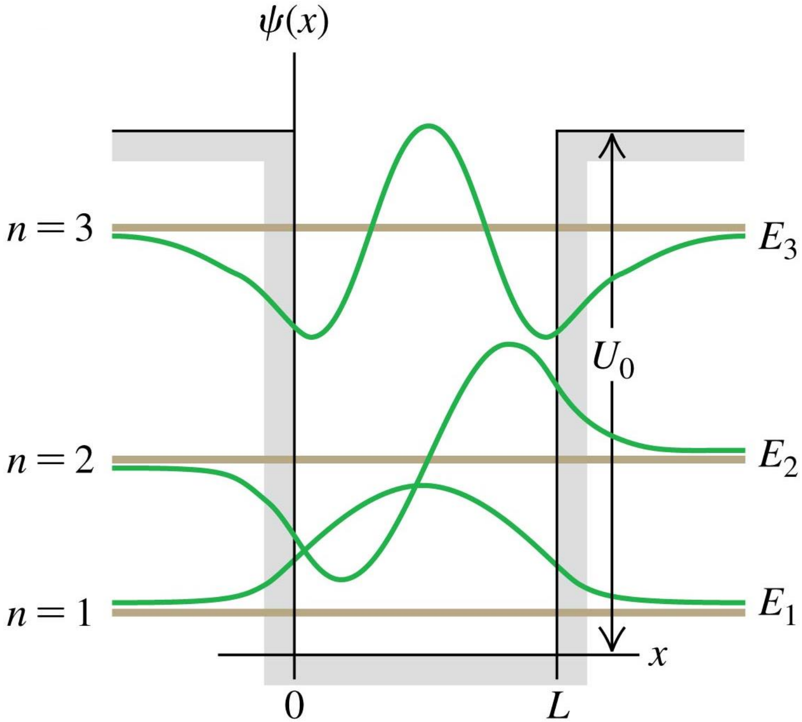
Particle in a finite potential well

- 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.



Q40.5

The first three wave functions ($n = 1$ through $n = 3$) for a finite square well are shown. The probability of finding the particle at $x > L$ is



A. least for $n = 1$.

B. least for $n = 2$.

C. least for $n = 3$.

D. the same (and nonzero) for $n = 1, 2$, and 3.

E. zero for $n = 1, 2$, and 3.

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

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

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.

Example 40.5: Outside a finite well

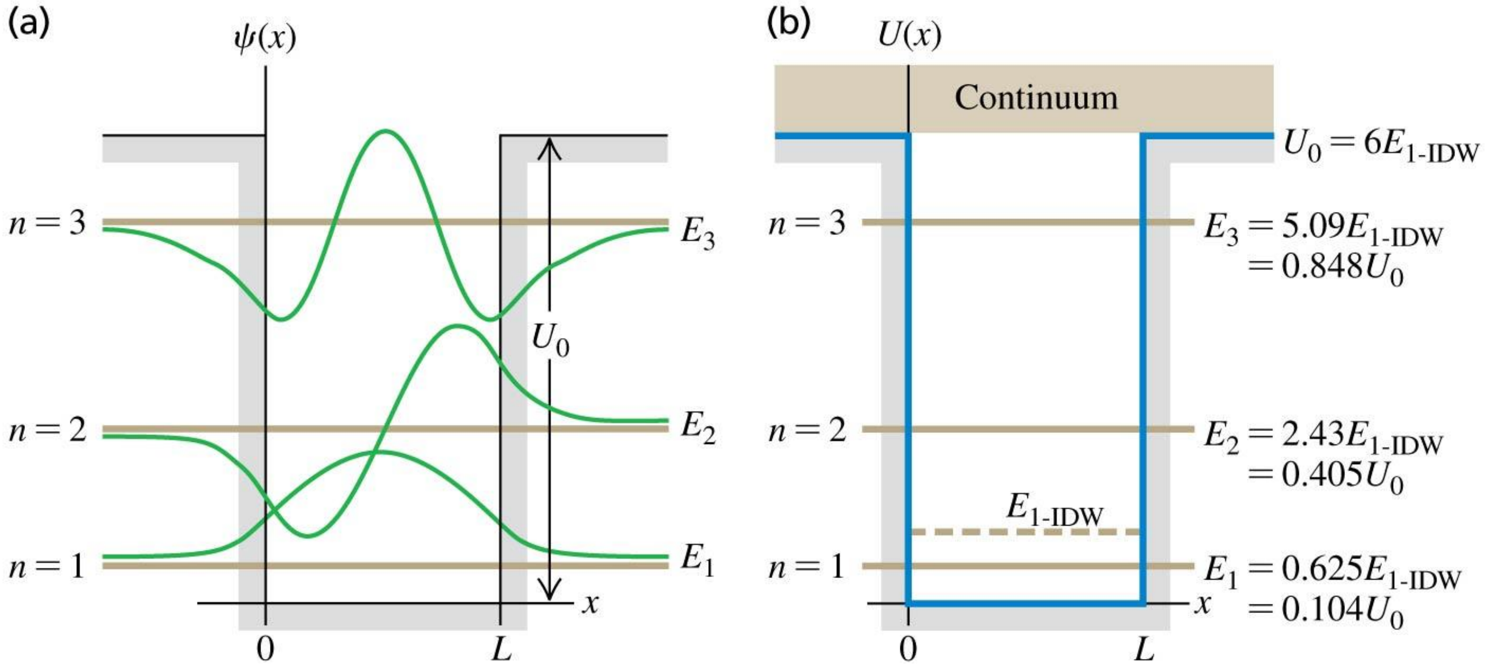
(a) Show that Eq. (40.40), $\psi(x) = Ce^{\kappa x} + De^{-\kappa x}$, is indeed a solution of the time-independent Schrödinger equation outside a finite well of height U_0. (b) What happens to $\psi(x)$ in the limit $U_0 \to \infty$?

(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.

EVALUATE: Our result in part (b) shows that the infinite square well is a *limiting case* of the finite well. We've seen many cases in Newtonian mechanics where it's important to consider limiting cases (such as Examples 5.11 and 5.13 in Section 5.2). Limiting cases are no less important in quantum mechanics.

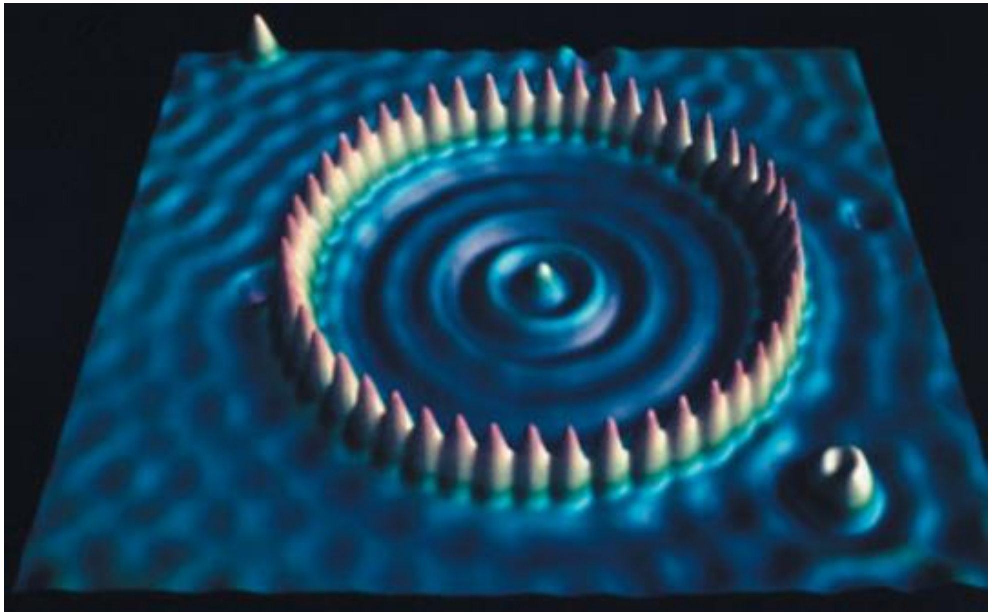
Comparing finite and infinite square wells

- Each energy level, including the ground level, is lower than that of the infinitely deep well (IDW)
- A well with finite depth only have a finite number of bound states (compared to infinite number for IDW). However, there is always at least one bound state, no matter how shallow the well is.
- As with IDW, no state has E = 0 as such a state would violate the uncertainty principle.



2D potential well

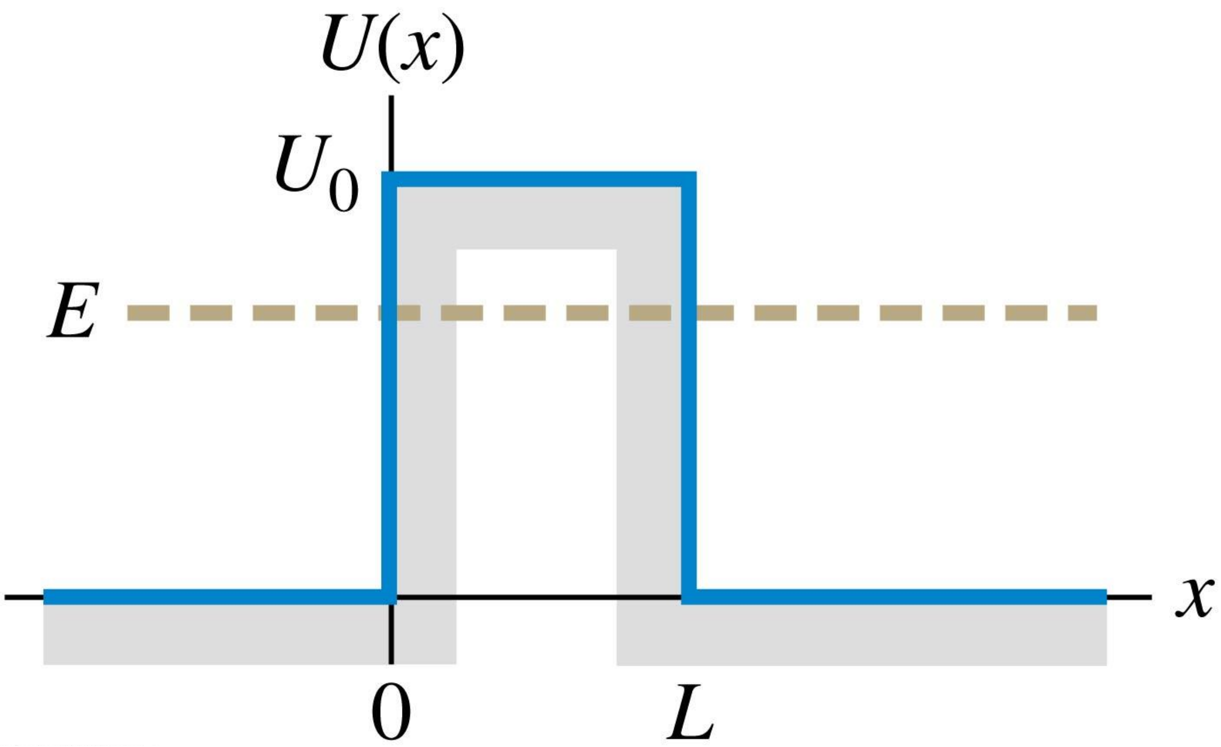
- 48 iron atoms (yellow peaks) were placed in a circle on a copper surface.
- The "elevation" at each point inside the circle indicates the electron density within the circle.



- The standing-wave pattern is very similar to the probability distribution function for a particle in a one-dimensional finite potential well.
- This image was made with a scanning tunneling microscope (STM).

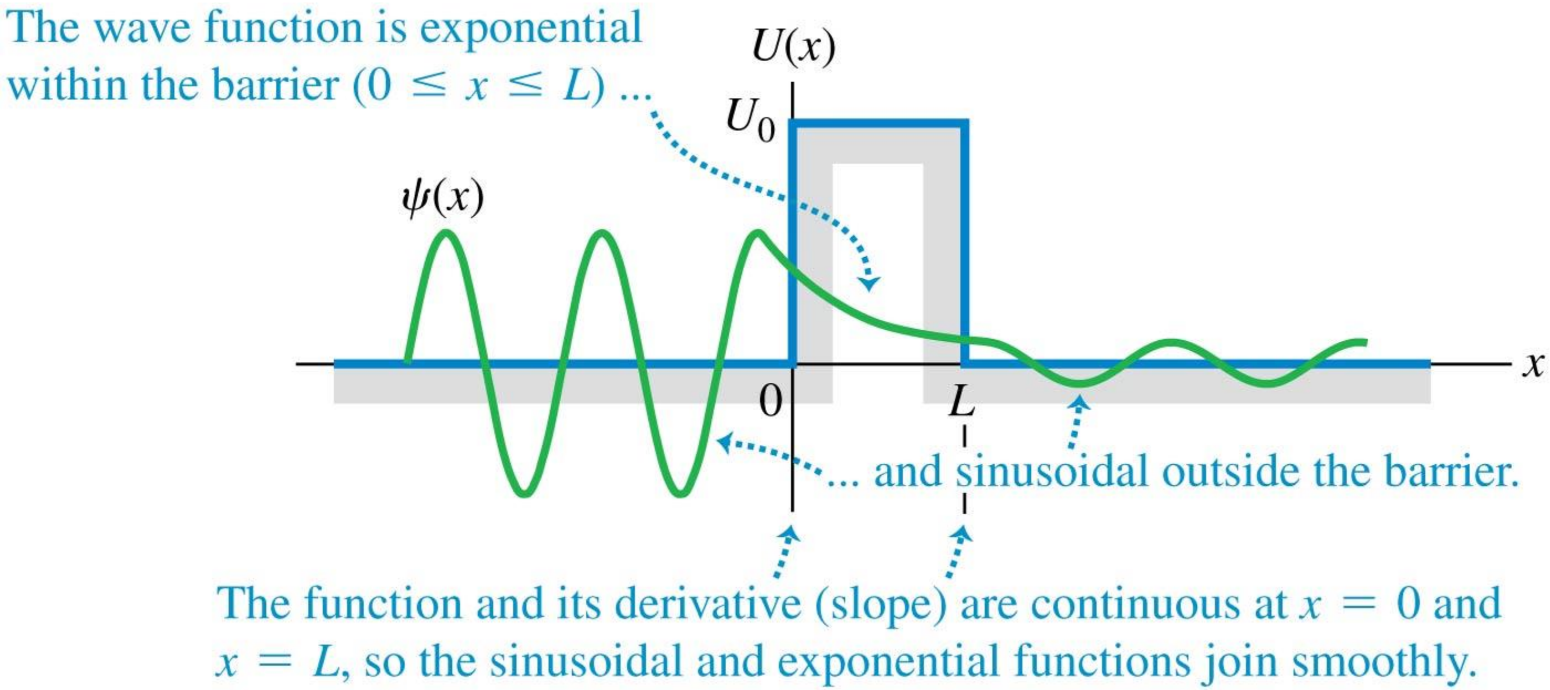
Potential barriers and tunneling

- 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

- 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.

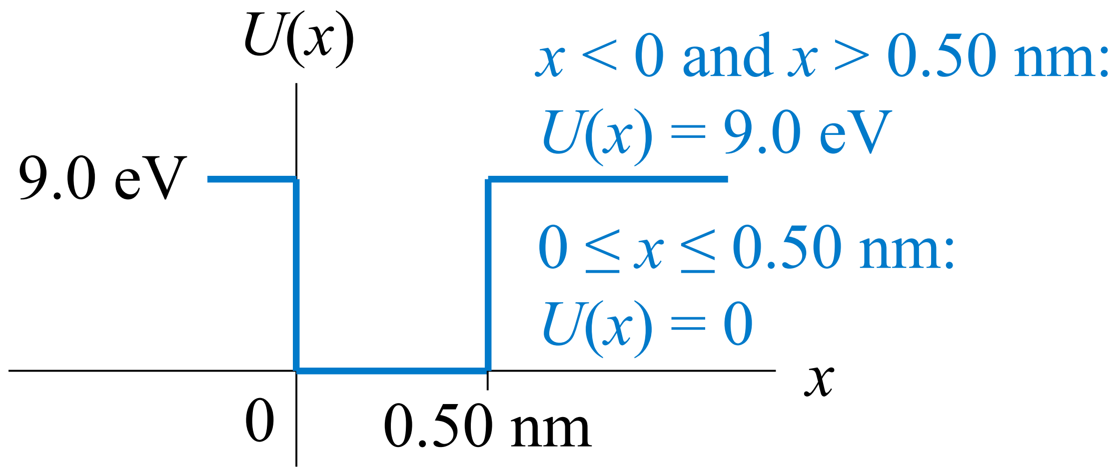


A quick question

- Is it possible for a particle undergoing tunneling to be found within the barrier rather than on either side of it?

Q40.6

The figure shows the potential-energy function $U(x)$ for a particle moving along the x-axis. Complete the sentence: "If the particle is in a bound state with energy $E = 0.94$ eV, the particle __________ be found at $x = -1.0$ nm according to Newtonian mechanics, and __________ be found at $x = -1.0$ nm according to quantum mechanics."



A. can, can

B. can, cannot

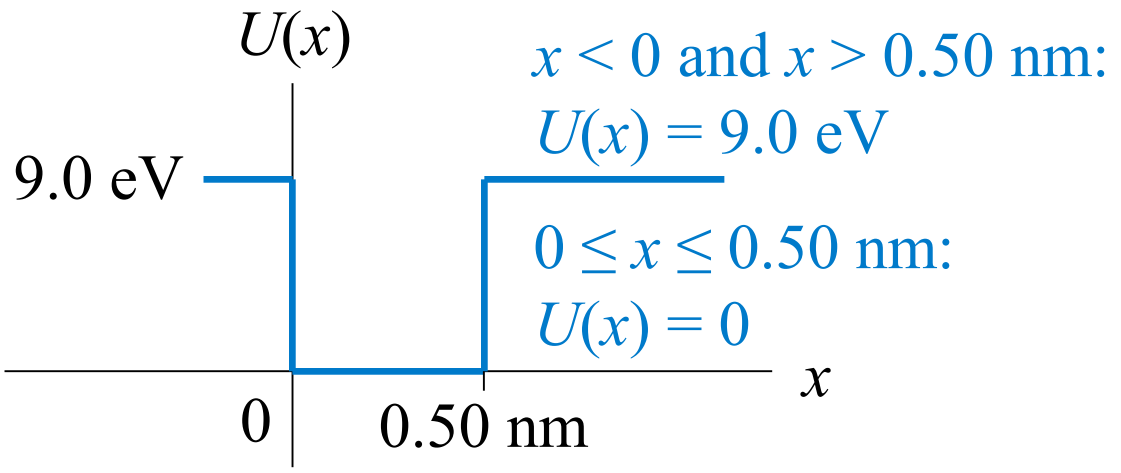
C. cannot, can

D. cannot, cannot

E. There are no quantum bound states for this $U(x)$.

Q40.7

The figure shows the potential-energy function $U(x)$ for a particle moving along the x-axis. Complete the sentence: "If the particle is in a state with energy E = 10.0 eV, the particle __________ be found at x = 0.25 nm according to Newtonian mechanics, and __________ be found at x = 0.25 nm according to quantum mechanics."



A. can, can

B. can, cannot

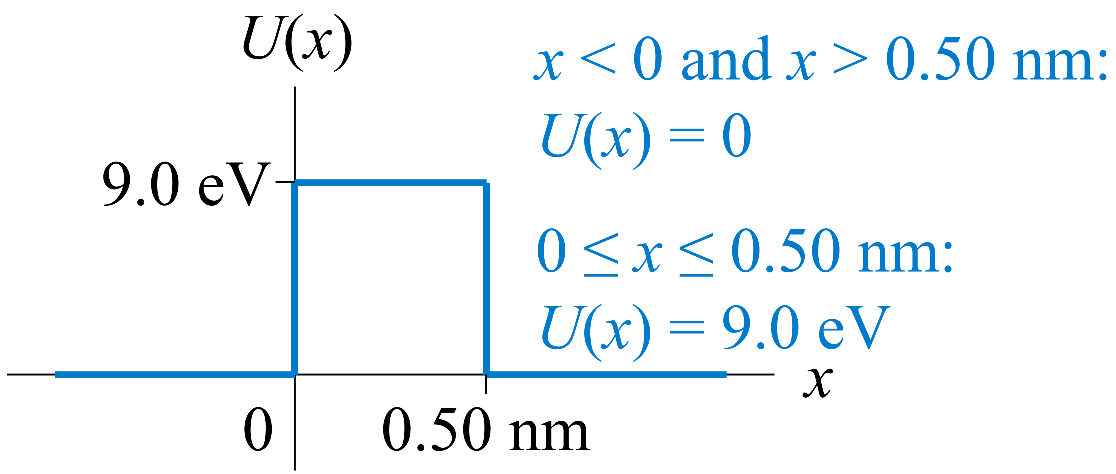
C. cannot, can

D. cannot, cannot

E. There are no quantum states with E = 10.0 eV for this $U(x)$.

Q40.8

The figure shows the potential-energy function $U(x)$ for a particle moving along the x-axis. Complete the sentence: "If the particle energy is $E = 3.0$ eV, the particle __________ be found at $x = 0.25$ nm according to Newtonian mechanics, and __________ be found at $x = 0.25$ nm according to quantum mechanics."



A. can, can

B. can, cannot

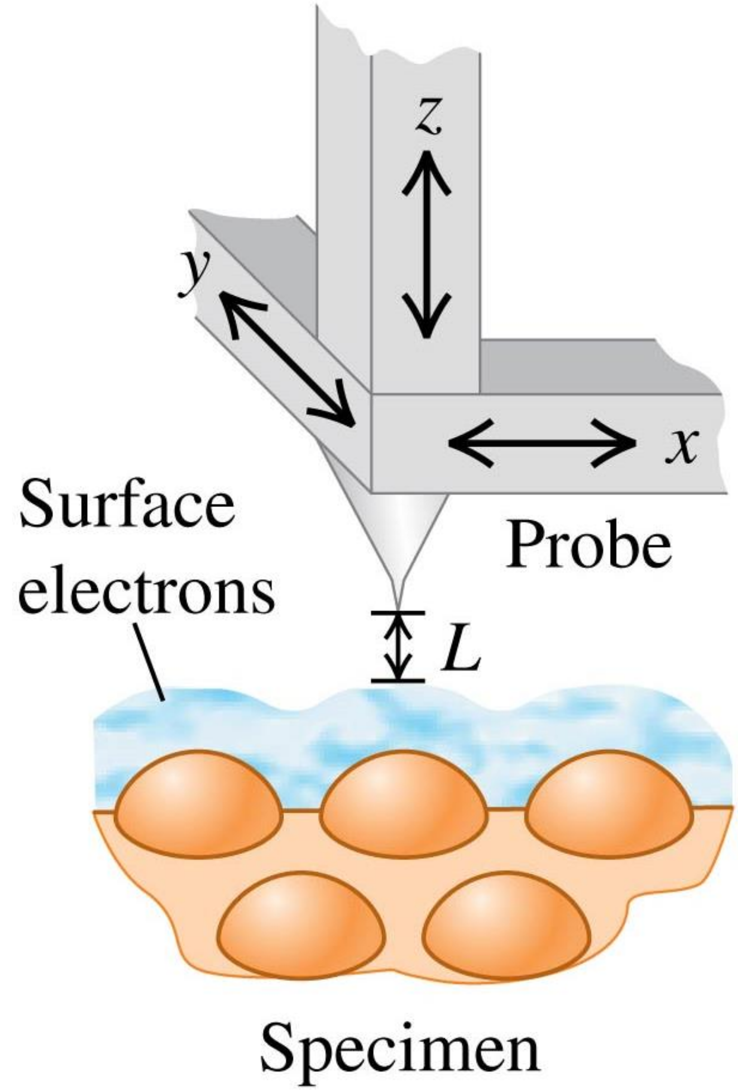
✔ C. cannot, can

D. cannot, cannot

E. There are no quantum states with $E = 3.0$ eV for this $U(x)$.

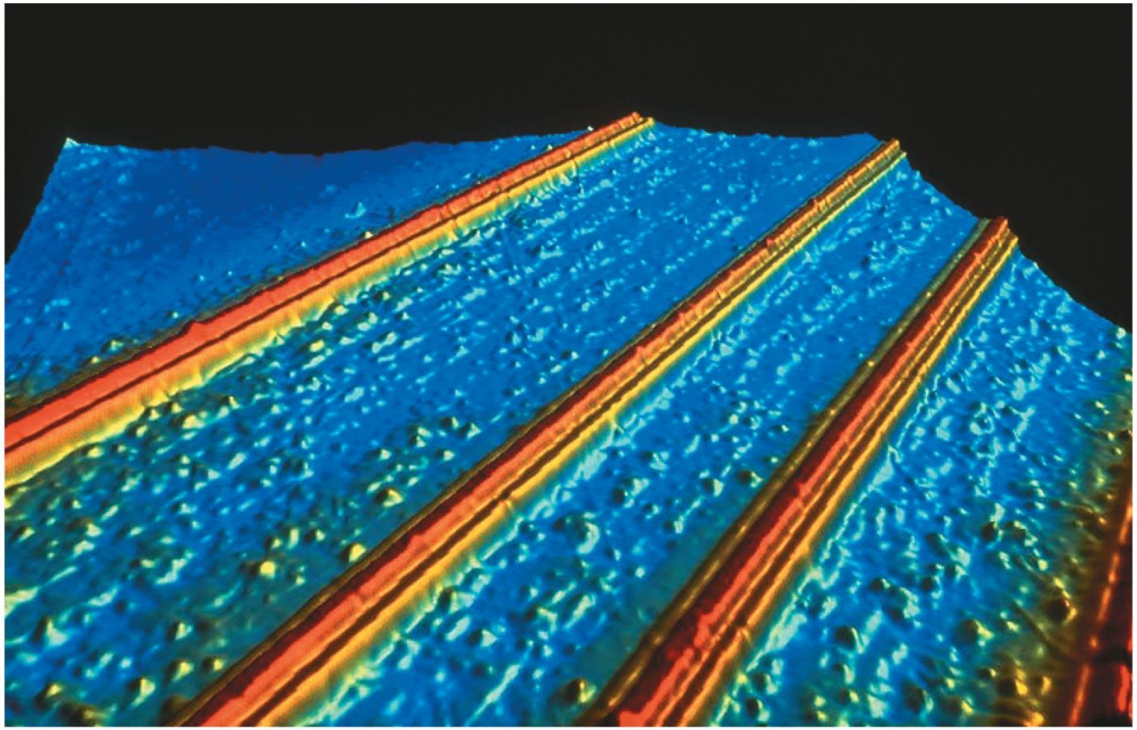
Scanning tunneling microscope (STM)

- 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.



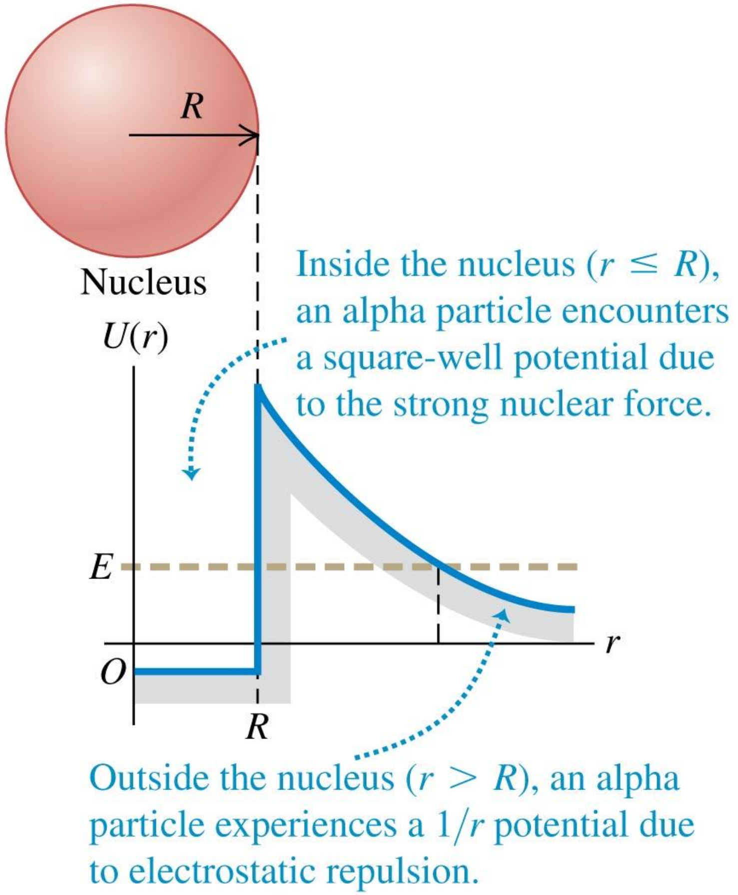
Scanning tunneling microscope (STM)

- 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.



Applications of tunneling

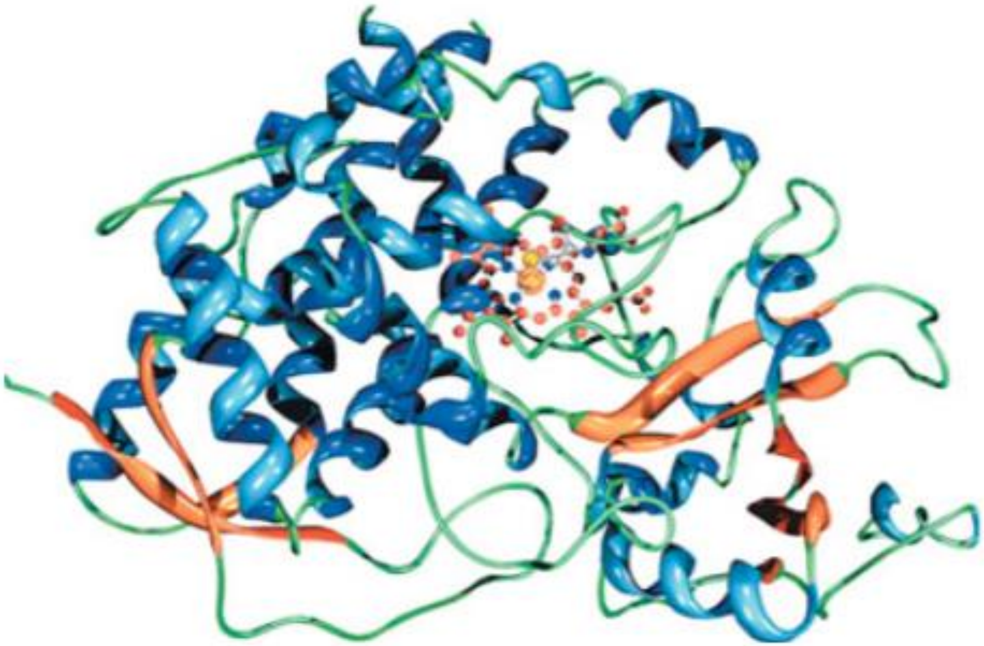
- Tunneling is of great importance in nuclear physics.
- An alpha particle trying to escape from a nucleus encounters a potential barrier that results from the combined effect of the attractive nuclear force and the electrical repulsion of the remaining part of the nucleus.
- To escape, the alpha particle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



Applications of tunneling

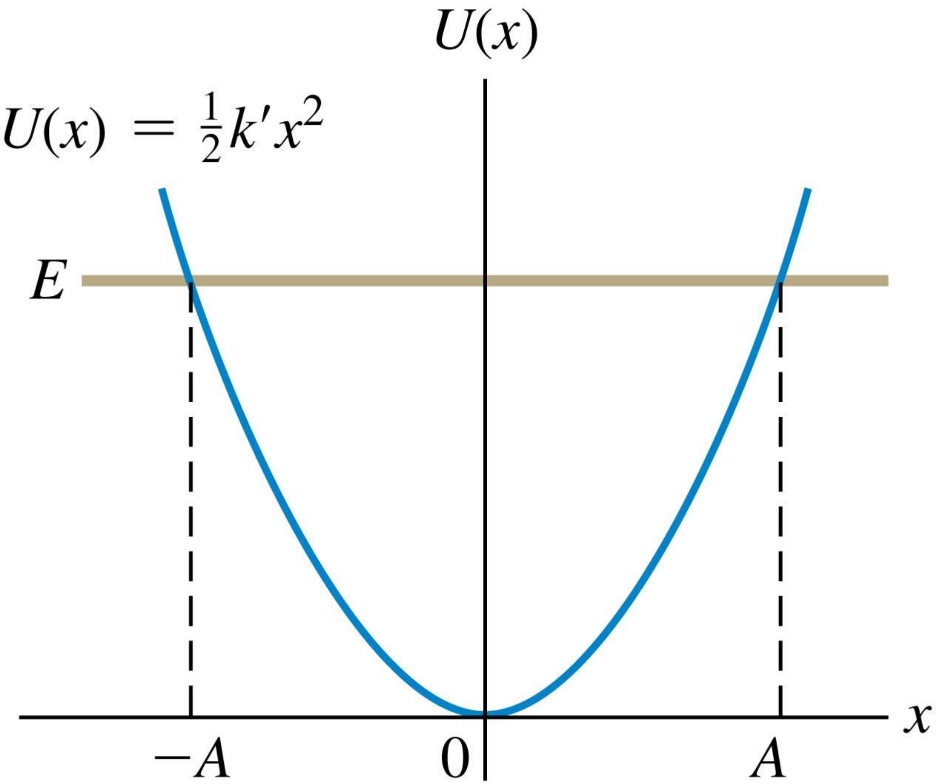
Application Electron Tunneling in Enzymes

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!



The harmonic oscillator

- 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

Quantum number

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

Planck's constant divided by 2π

Particle's mass

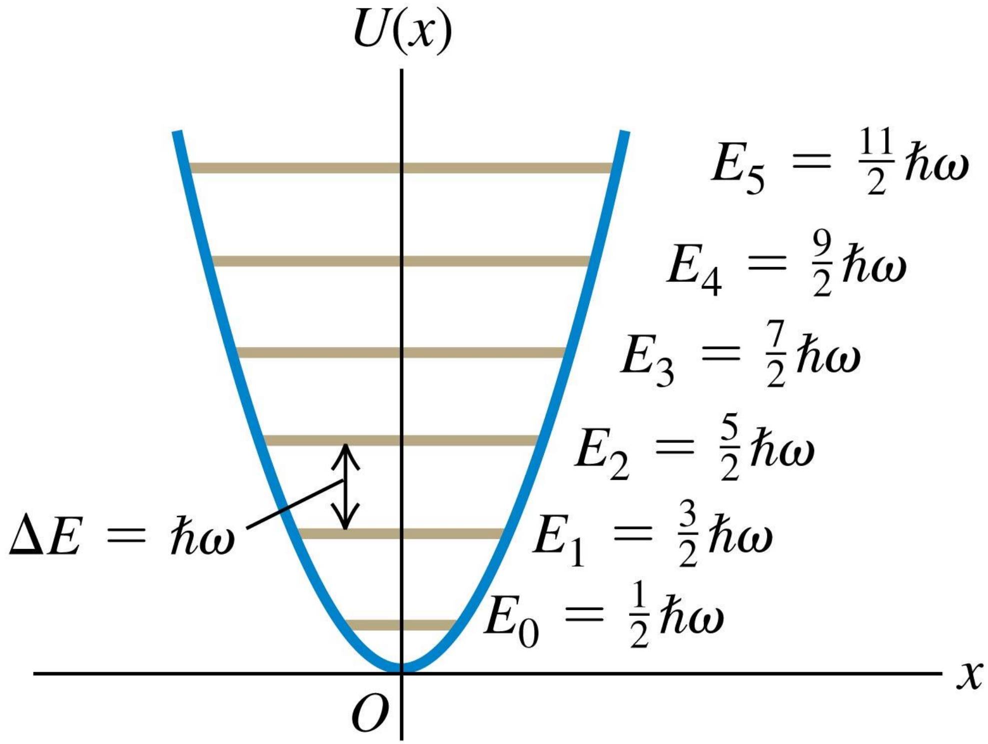
Force constant

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, $U = ½\, k'x^2$ increases without bound.

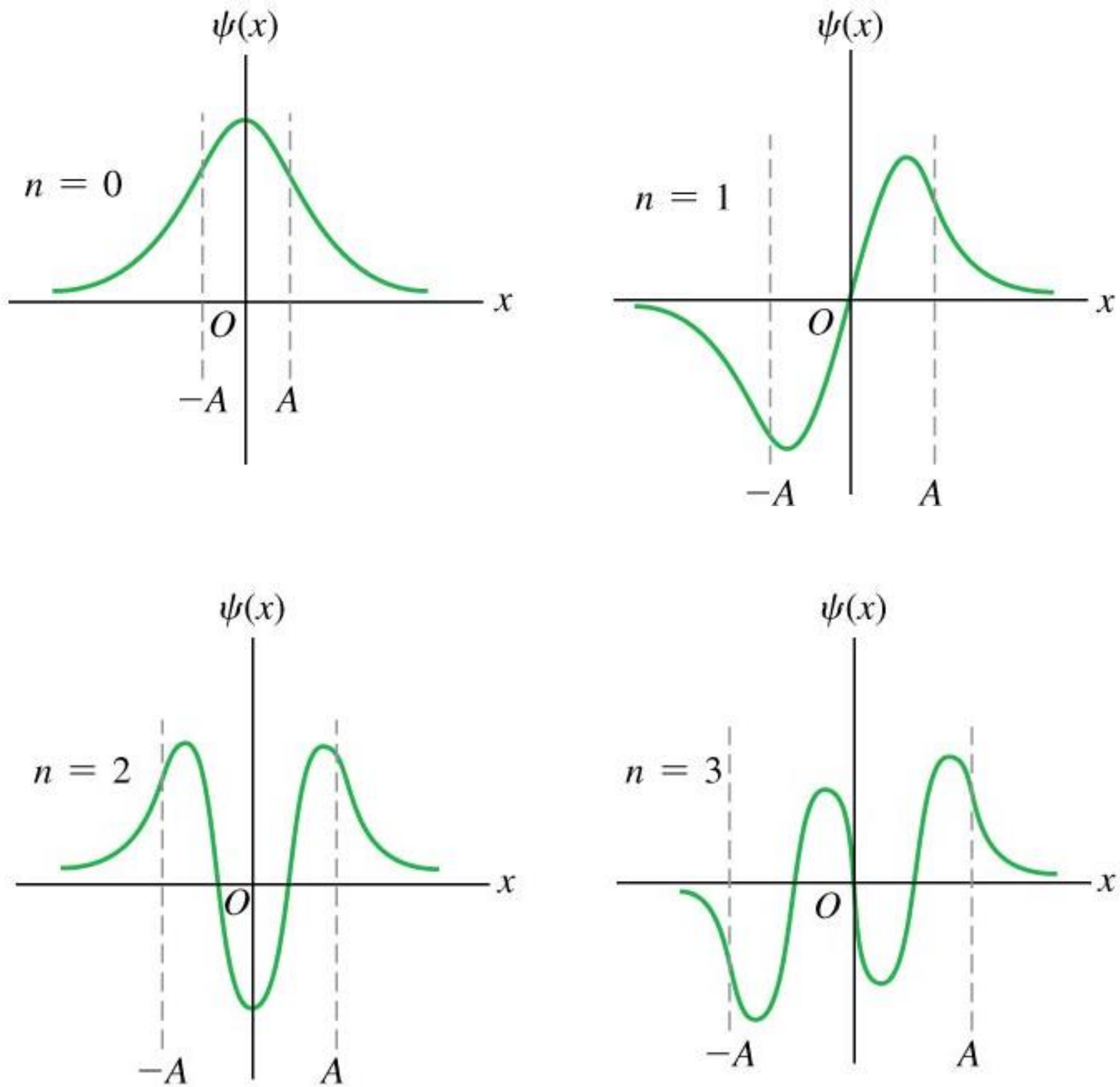
The harmonic oscillator

- 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.



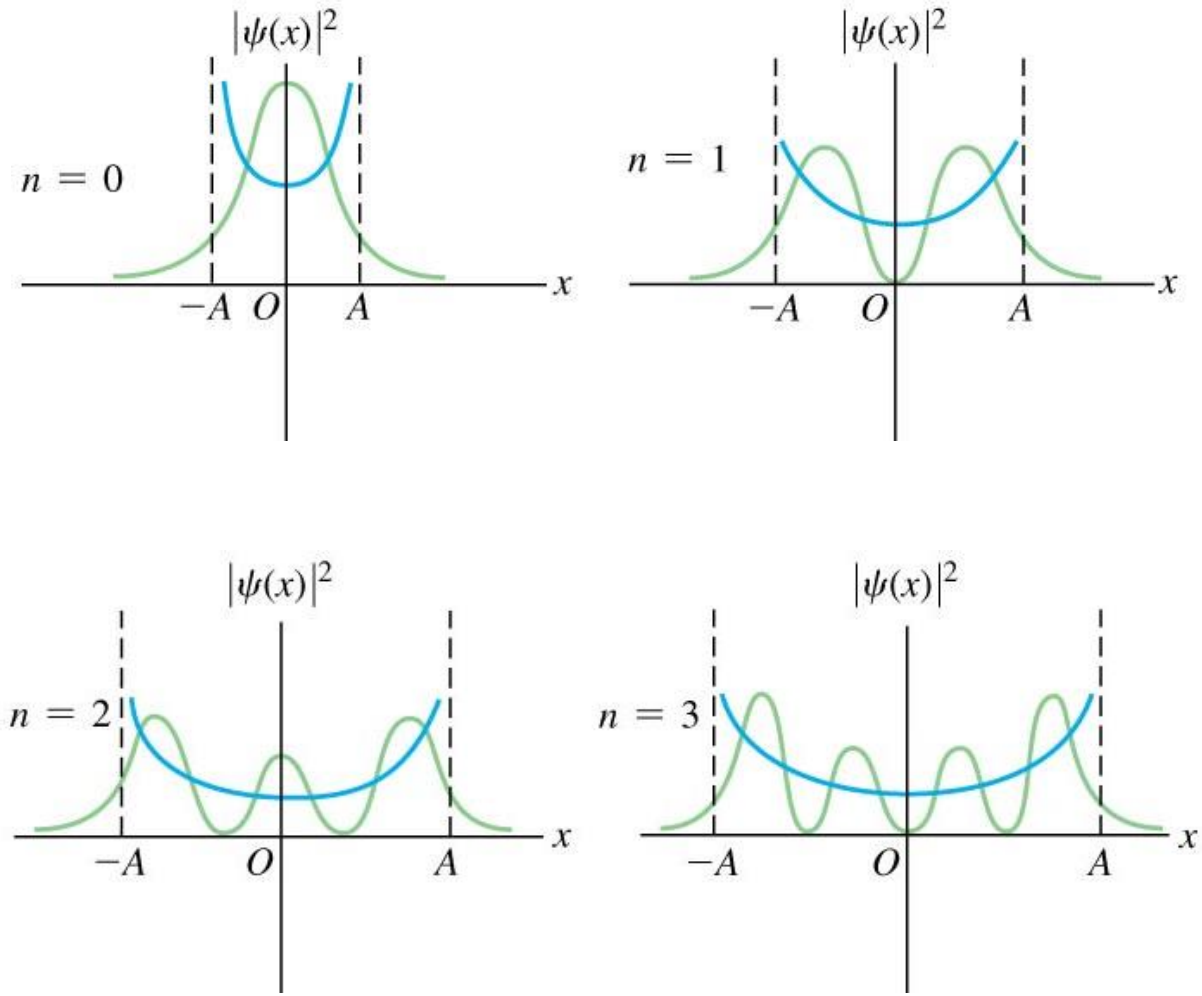
Wave functions for the harmonic oscillator

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



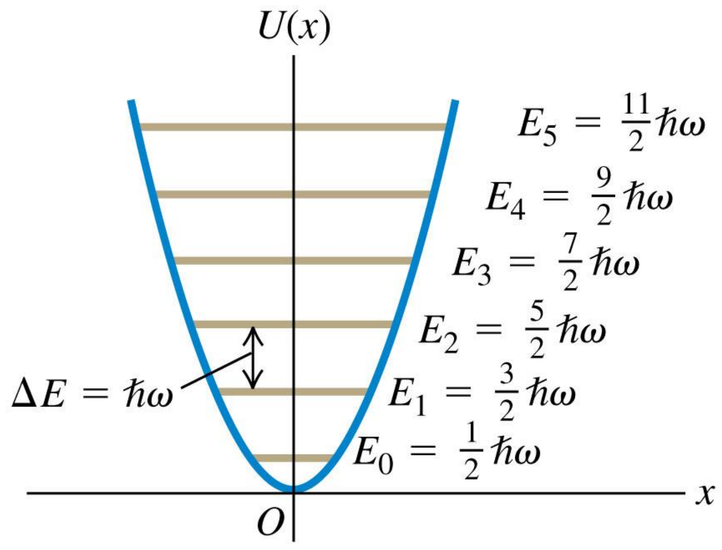
Probability distributions for the harmonic oscillator

- 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.



Q40.10

The figure shows the first six energy levels of a quantum-mechanical harmonic oscillator. The corresponding wave functions



A. are nonzero outside the region allowed by Newtonian mechanics.

B. do not have a definite wavelength.

C. are all equal to zero at $x = 0$.

D. both A and B are true.

E. all of A, B, and C are true.

Q40.11

A particle in a potential well emits a photon when it drops from the $n = 3$ energy level to the $n = 2$ energy level. The particle then emits a second photon when it drops from the $n = 2$ energy level to the $n = 1$ energy level. The first photon has the same energy as the second photon. What kind of potential well could this be?

A. an infinitely deep square potential well (particle in a box)

B. a finite square well

C. a harmonic oscillator

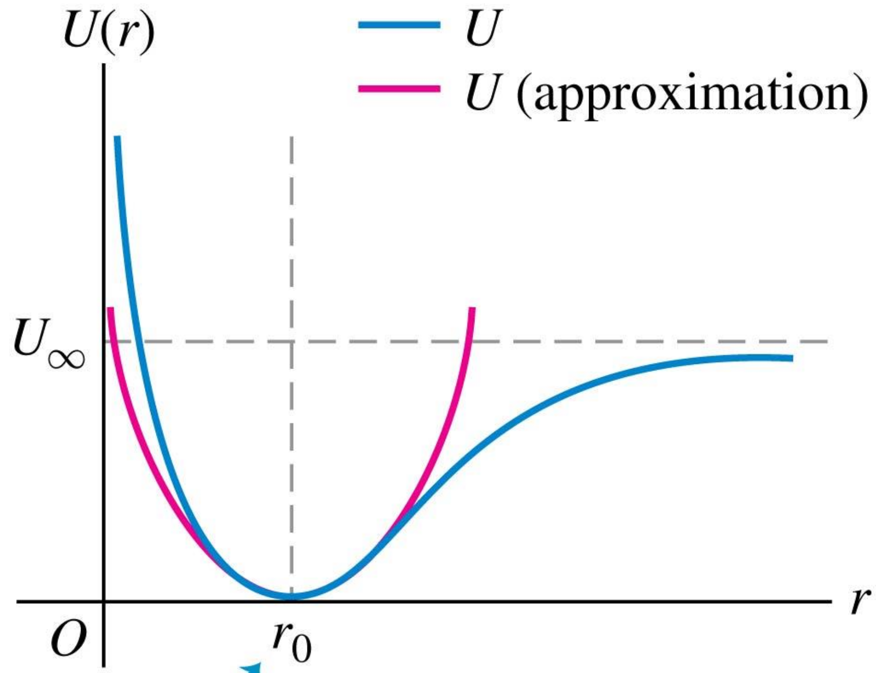
D. two of A, B, and C

E. all three of A, B, and C

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.

Example 40.8: Vibration in a crystal

A sodium atom of mass 3.82×10^{-26} kg vibrates within a crystal. The potential energy increases by 0.0075 eV when the atom is displaced 0.014 nm from its equilibrium position. Treat the atom as a harmonic oscillator. (a) Find the angular frequency of the oscillations according to Newtonian mechanics. (b) Find the spacing (in electron volts) of adjacent vibrational energy levels according to quantum mechanics. (c) What is the wavelength of a photon emitted as the result of a transition from one level to the next lower level? In what region of the electromagnetic spectrum does this lie?

EXECUTE: We are given that $U = 0.0075\ \text{eV} = 1.2 \times 10^{-21}\ \text{J}$ when $x = 0.014 \times 10^{-9}$ m, so we can solve $U = \frac{1}{2}k'x^2$ for k':

$$k' = \frac{2U}{x^2} = \frac{2(1.2 \times 10^{-21}\ \text{J})}{(0.014 \times 10^{-9}\ \text{m})^2} = 12.2\ \text{N/m}$$

(a) The Newtonian angular frequency is

$$\omega = \sqrt{\frac{k'}{m}} = \sqrt{\frac{12.2\ \text{N/m}}{3.82 \times 10^{-26}\ \text{kg}}} = 1.79 \times 10^{13}\ \text{rad/s}$$

(b) From Eq. (40.46) and Fig. 40.25, the spacing between adjacent energy levels is

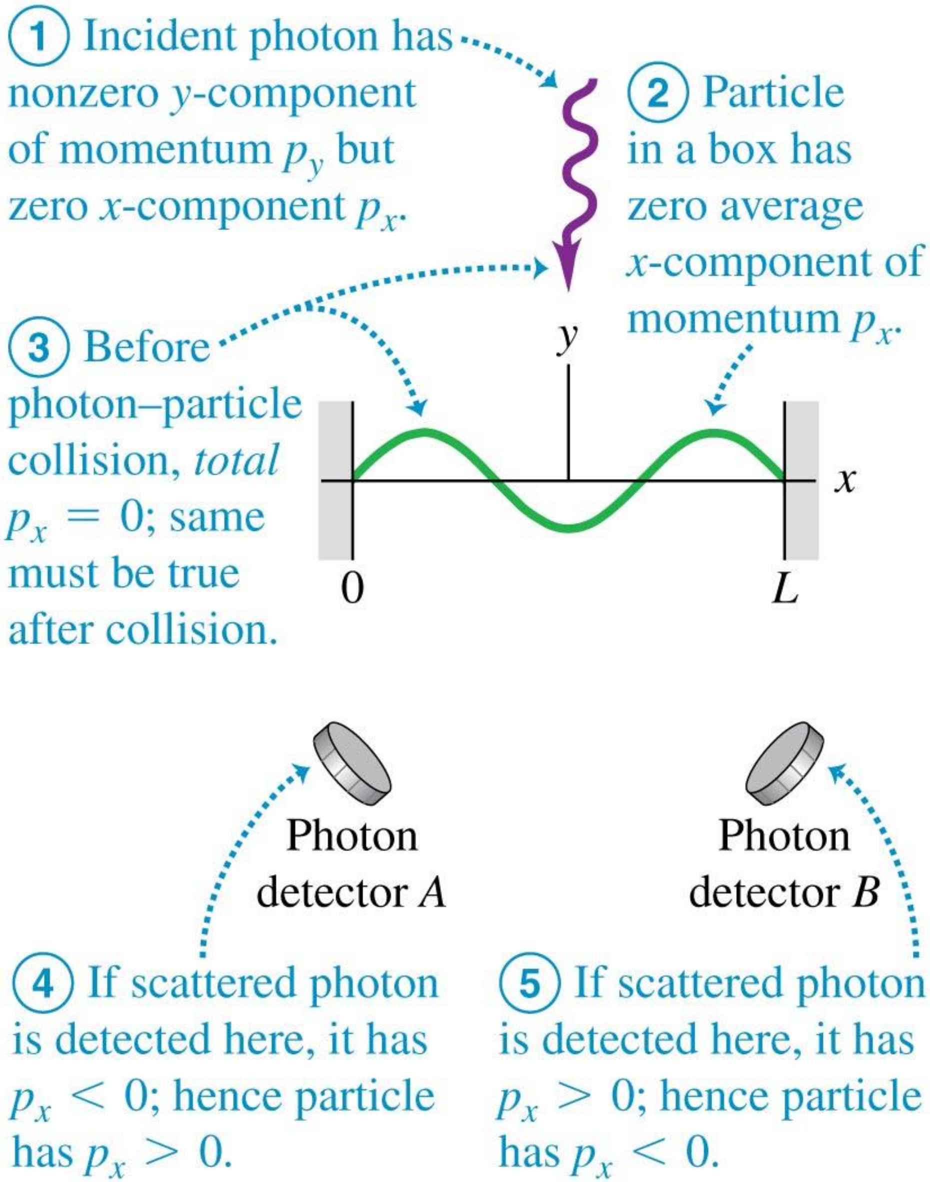
$$\begin{aligned}\hbar\omega &= (1.054 \times 10^{-34}\ \text{J}\cdot\text{s})(1.79 \times 10^{13}\ \text{s}^{-1})\\ &= 1.88 \times 10^{-21}\ \text{J}\left(\frac{1\ \text{eV}}{1.602 \times 10^{-19}\ \text{J}}\right) = 0.0118\ \text{eV}\end{aligned}$$

(c) The energy E of the emitted photon is equal to the energy lost by the oscillator in the transition, 0.0118 eV. Then

$$\begin{aligned}\lambda &= \frac{hc}{E} = \frac{(4.136 \times 10^{-15}\ \text{eV}\cdot\text{s})(3.00 \times 10^{8}\ \text{m/s})}{0.0118\ \text{eV}}\\ &= 1.05 \times 10^{-4}\ \text{m} = 105\ \mu\text{m}\end{aligned}$$

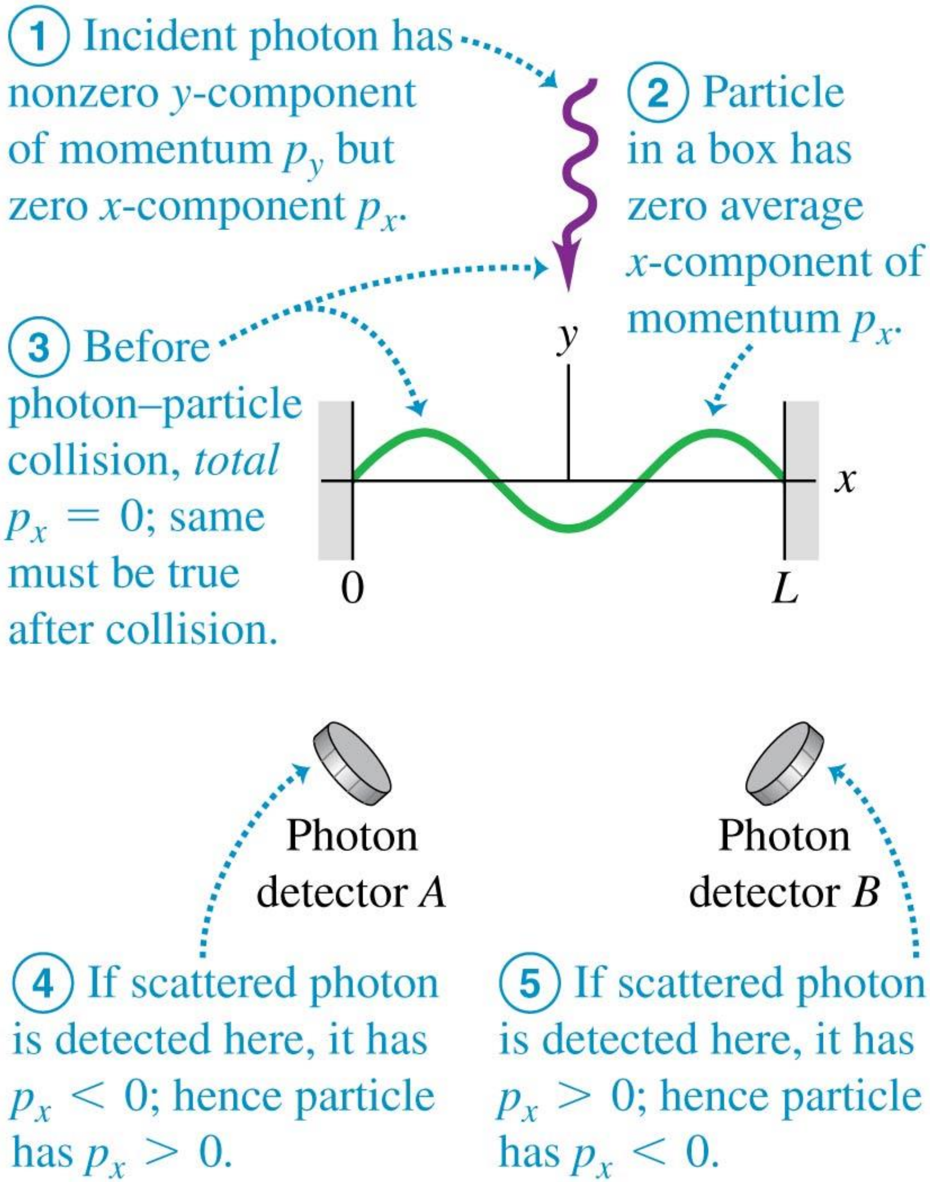
This photon wavelength is in the infrared region of the spectrum.

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.
- **Measuring a physical property of a system can (irreversibly) change the wave function of that system.**

Measurement in quantum mechanics



- Wave function: A[exp(ikx)- exp(-ikx)]
- Before the measurement: the system is in a **linear superposition** of two **eigenstates**: exp(ikx) and exp(-ikx)
- After the measurement, the system **collapses** to one of its eigenstates
- (But we cannot predict *which one* it is going to collapse into before we actually make the measurement; we only know the relative probabilities.)

Q40.12

A particle in a box is described by a wave function that is a combination of the $n = 1$ stationary state [energy E_1, time-independent wave function $\psi_1(x)$] and the $n = 2$ stationary state [energy E_2, time-independent wave function $\psi_2(x)$]:

$$\Psi(x,t) = C\psi_1(x)e^{-iE_1t/\hbar} + D\psi_2(x)e^{-iE_2t/\hbar}$$

Here C and D are constants. If you measure the energy of this particle, the result of your measurement is *guaranteed* to be

A. E_1.

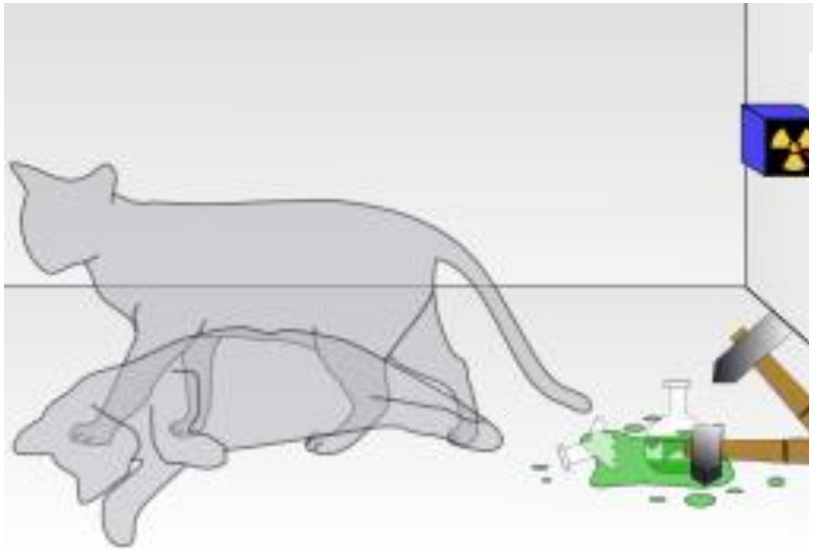
B. E_2.

C. $(E_1 + E_2)/2$.

D. a value between E_1 and E_2 that depends on C and D.

E. none of the above.

Schrödinger's cat



Quantum superposition of distinct macroscopic states

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In 1935, Schrödinger[1] attempted to demonstrate the limitations of quantum mechanics using a thought experiment in which a cat is put in a quantum superposition of alive and dead states. The idea remained an academic curiosity until the 1980s when it was proposed[2–4] that, under suitable conditions, a macroscopic object with many microscopic degrees of freedom could behave quantum mechanically, provided that it was sufficiently decoupled from its environment. Although much progress has been made in demonstrating the macroscopic quantum behaviour of various systems such as superconductors[5–9], nanoscale magnets[10–12], laser-cooled trapped ions[13], photons in a microwave cavity[14] and C_{60} molecules[15], there has been no experimental demonstration of a quantum superposition of truly macroscopically distinct states. Here we present experimental evidence that a superconducting quantum interference device (SQUID) can be put into a superposition of two magnetic-flux states: one corresponding to a few microamperes of current flowing clockwise, the other corresponding to the same amount of current flowing anticlockwise.

Quantum Communication: The Micius “墨子號”

The New York Times

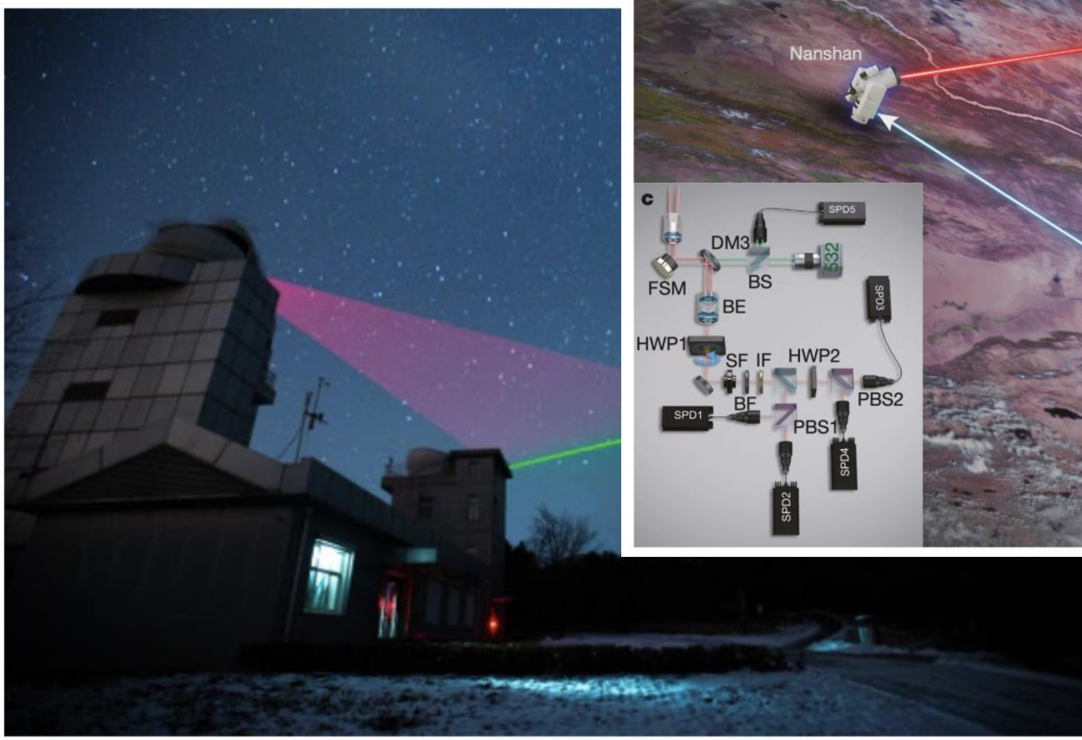
China Launches Quantum Satellite in Bid to Pioneer Secure Communications

By EDWARD WONG AUG. 16, 2016

BEIJING — China launched the world’s first quantum communications satellite from the Gobi Desert early Tuesday, a major step in the country’s bid to be at the forefront of quantum research, which could lead to new, completely secure methods of transmitting information.

Researchers hope to use the satellite to beam communications from space to earth with quantum technology, which employs photons, or particles of light. That type of communication could prove to be the most secure in the world, invulnerable to hacking. Scientists and security experts in many countries are studying the technology.

Quantum Communication: The Micius “墨子號”



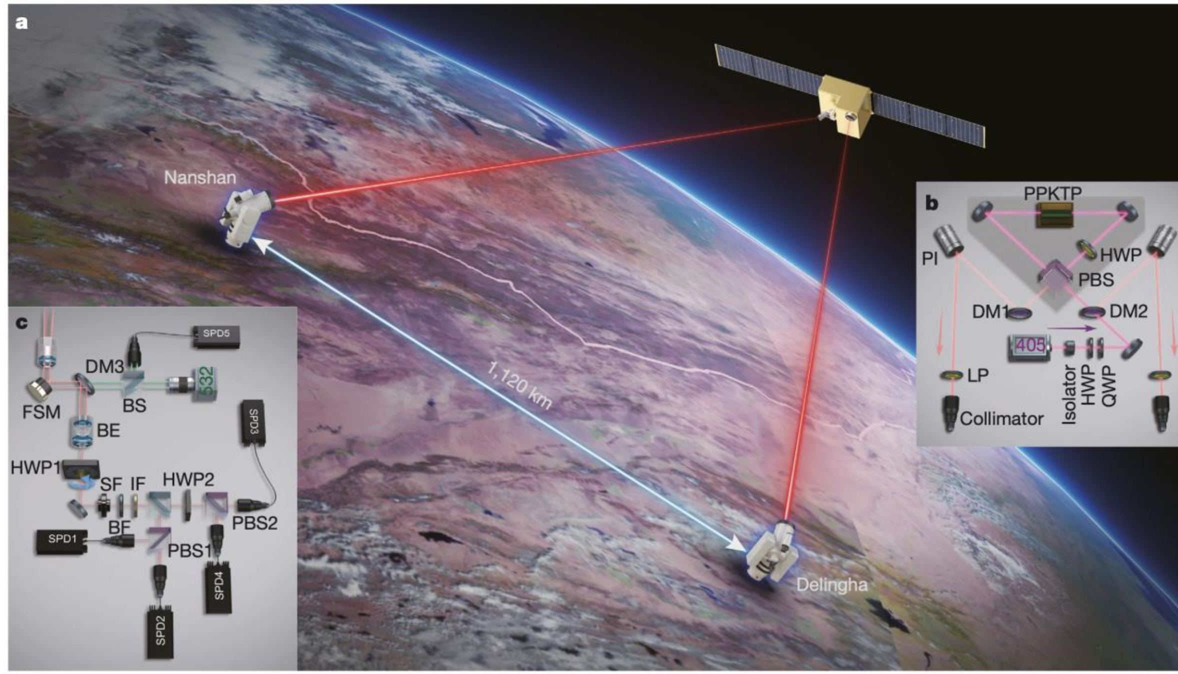


Photo taken on Nov. 26, 2016 shows a satellite-to-earth link established between quantum satellite "Micius" and the quantum communication ground station in Xinglong, north China's Hebei Province.
Credit: Jin Liwang *Alamy*

Some extras about the Schrödinger equation

Bust of Schrödinger, in the courtyard arcade of the main building, University of Vienna, Austria

Tombstone of Annemarie and Erwin Schrödinger in Tirol, Austria

You can read more about the history of the Schrödinger equation [here](#).

Some extras about Schrödinger

Original cover to Erwin Schrodinger's famous 1944 Dublin lecture *What is Life?*, the book that inspired James Watson to discover DNA (1953) and that initiated the famous "life feeds on negative entropy" supposition.