Quantum Mechanics

Wave functions and the Schrodinger equation

Particles behave like waves, so they can be described with a wave function $\Psi(x,y,z,t)$

A stationary state has a definite energy, and can be written as

$$\Psi(x, y, z, t) = \psi(x, y, z)\, e^{-iEt/\hbar} \qquad (39.14)$$

(time-dependent wave function for a stationary state)

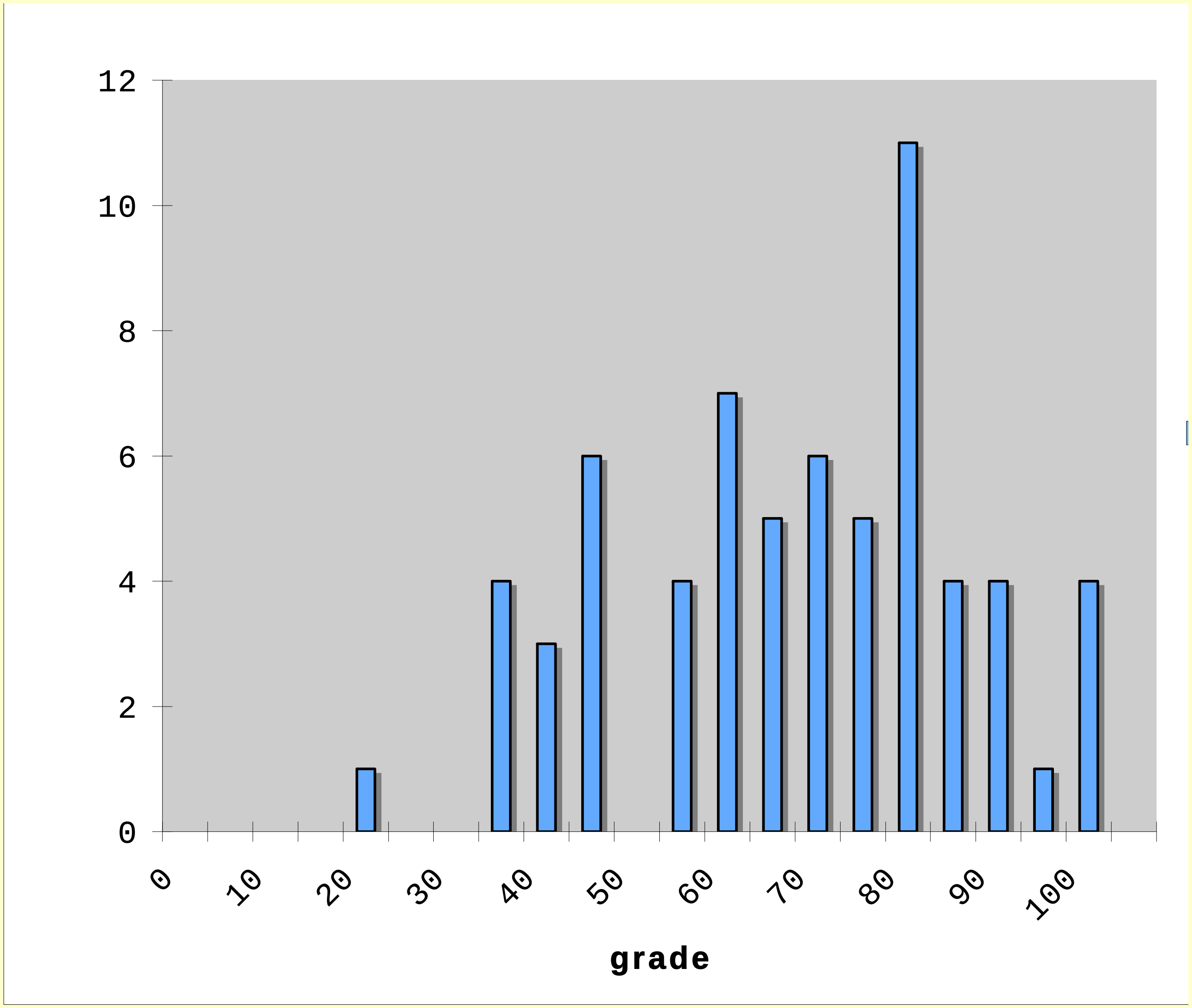
$\Psi^*\Psi = |\Psi|^2$ = "Probability distribution function"

$|\Psi|^2\, dV$ = probability of finding a particle near a given point x,y,z at a time t

For a stationary state,

- $\Psi^*\Psi$ is independent of time
- $\Psi^*\Psi = |\psi(x,y,z)|^2$

Grade distribution function



The Schrodinger Equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x) \qquad (39.18)$$

(one-dimensional Schrödinger equation)

Solving this equation will give us

- the possible energy levels of a system (such as an atom)
- The probability of finding a particle in a particular region of space

It's hard to solve this equation. Therefore, our approach will be to learn about a few of the simpler situations and their solutions.

The Schrodinger equation:

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

Kinetic energy	+	Potential energy	=	Total energy

For a given U(x),

- what are the possible $\psi(x)$?
- What are the corresponding E?

For a free particle, U(x) = 0, so

$$\psi(x) = Ae^{ikx}$$

Where k = 2π / λ
= anything real

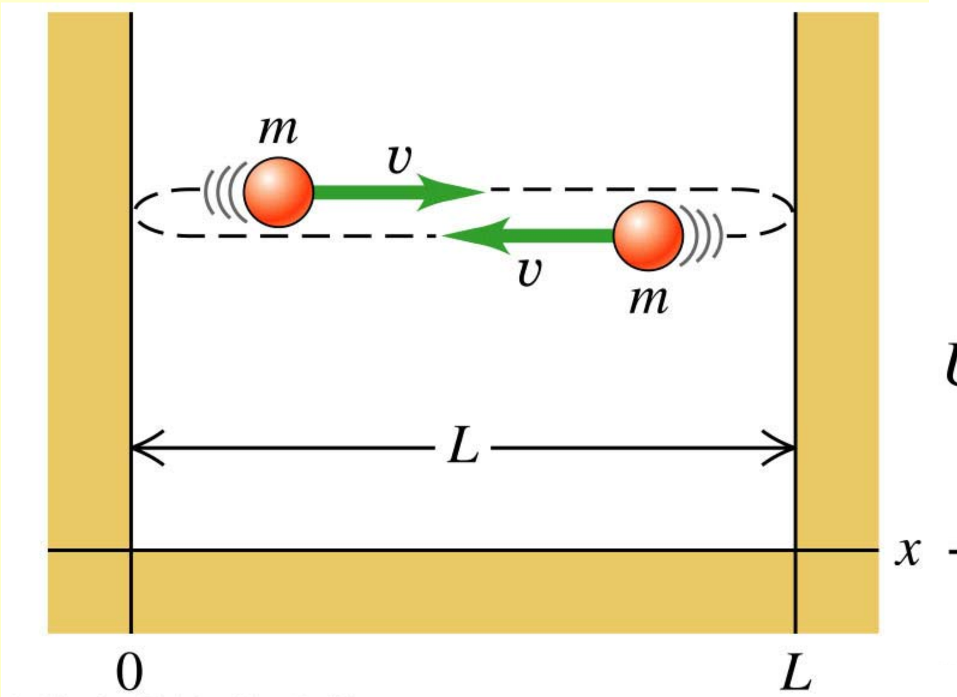
$$E = \frac{\hbar^2 k^2}{2m}$$

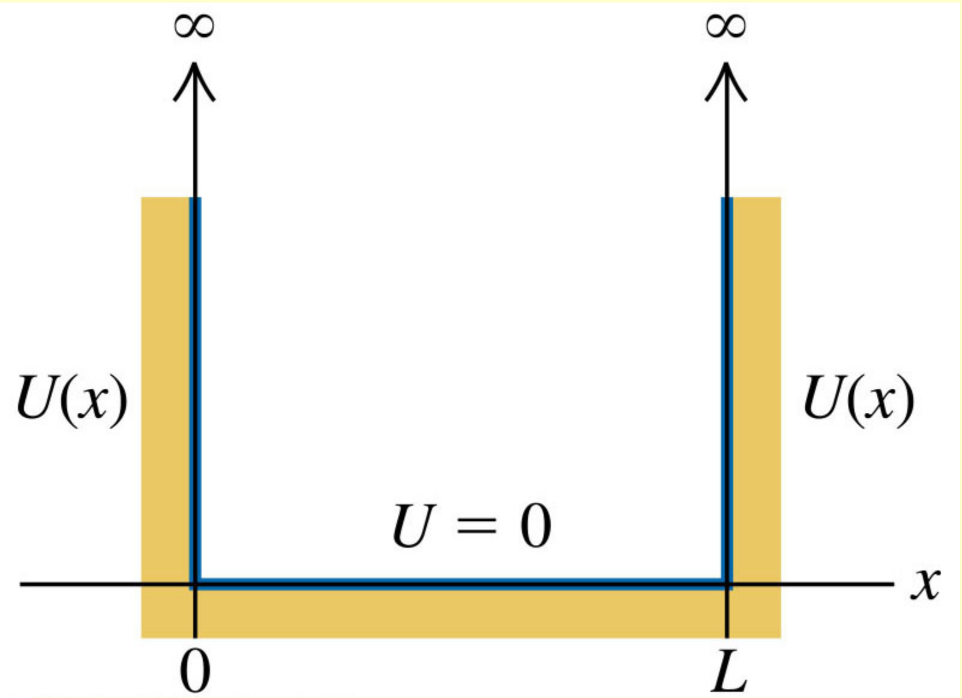
= any value from
0 to infinity

Momentum: $p = \hbar k$

The free particle can be found anywhere, with equal probability

Particle in a box





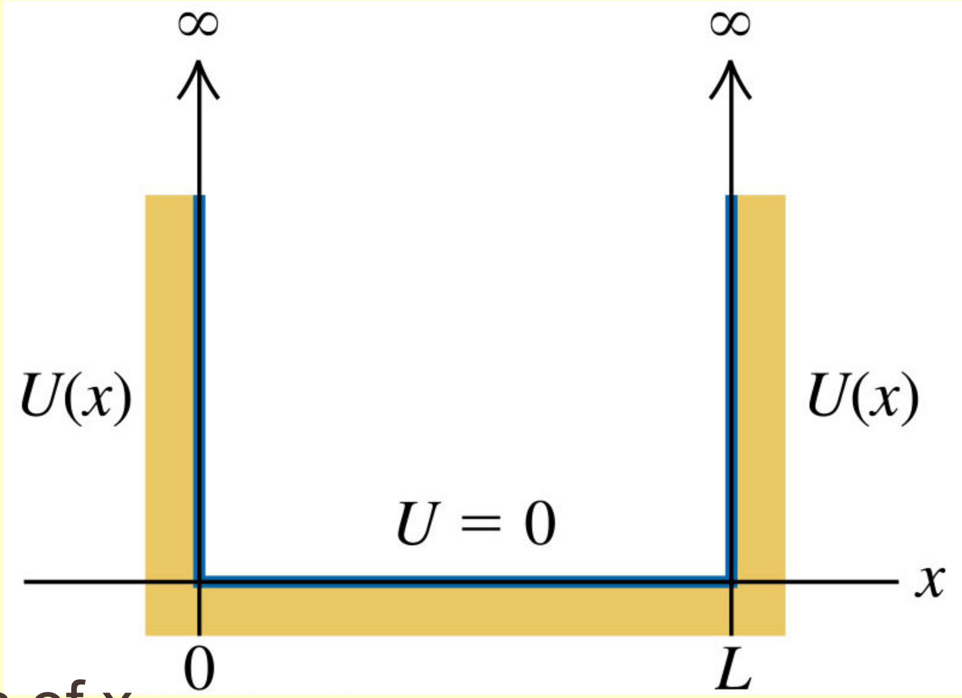
Rigid walls
Newton's view

Potential energy
function U(x)

The particle in a box is not free, it is "bound" by U(x)

<u>Examples:</u> An electron in a long molecule or in a straight wire

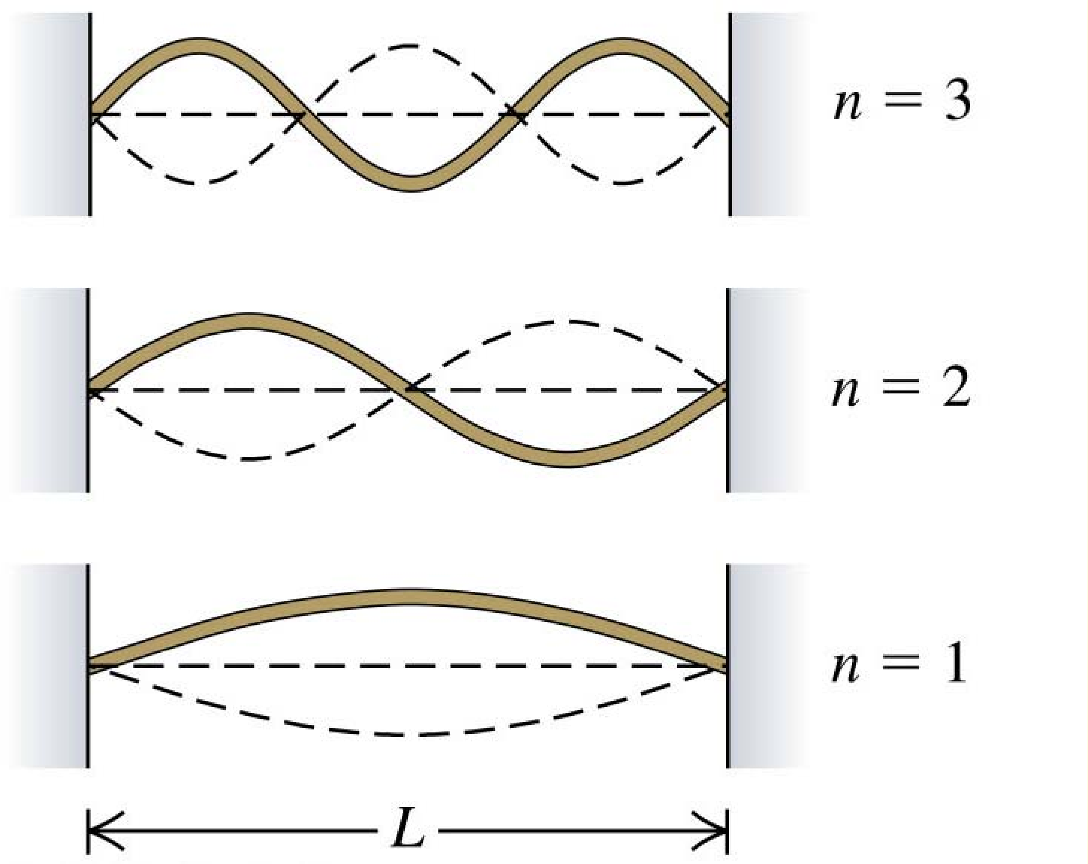
To be a solution of the SE, ψ(x) has to be continuous everywhere, except where U(x) has an infinite discontinuity



"Boundary conditions":
ψ(x) = 0 at x=0, L and all values of x outside this box, where U(x) = infinite

Solutions to the S.E. for the particle in a box

$d\psi/dx$ also has to be continuous everywhere, (except where $U(x)$ has an infinite discontinuity) because you need to find $d^2\psi/dx^2$



Normal modes of a vibrating string!

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

From 0 < x < L, U(x) = 0, so in this region, ψ(x) must satisfy:

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

Same as a free particle?!?!?!?!?

You may be tempted to conclude that

$$\psi(x) = Ae^{ikx}$$

, the solution for a free particle, is a possible solution for the bound one too.

WRONG!!!!

Why not?

The above $\psi(x)$ does NOT satisfy the boundary conditions that $\psi(x) = 0$ at x=0 and x=L.

So what is the solution then?

Try the next simplest solution, a superposition of two waves

$$\psi(x) = A_1 e^{ikx} + A_2 e^{-ikx}$$

The energy again is $E = \dfrac{\hbar^2 k^2}{2m}$

Rewrite $\psi(x)$ *with* sin *and* cos

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

Choose values of k and λ that satisfy the boundary conditions:

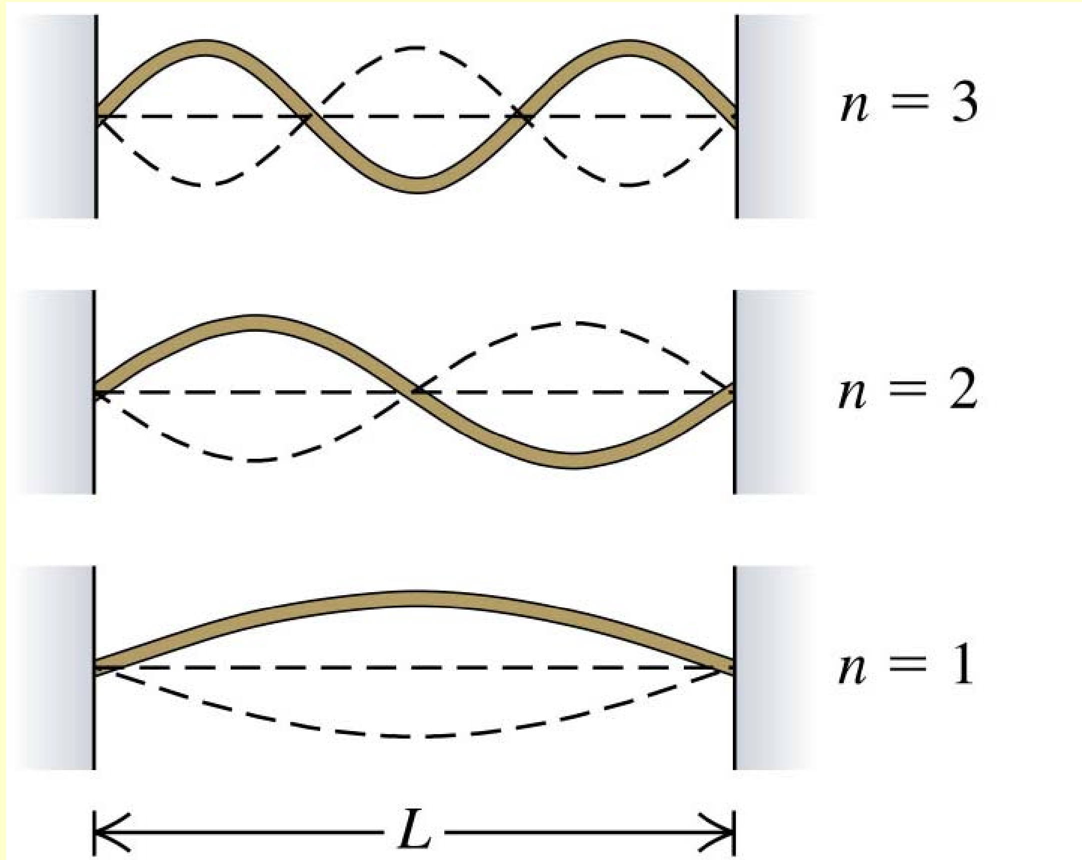
$\psi(x) = 0$ when $x=0$ and $x=L$

$k = n\pi / L$ $\lambda = 2\pi / k = 2L / n$

Where $n = 1, 2, 3, \ldots$

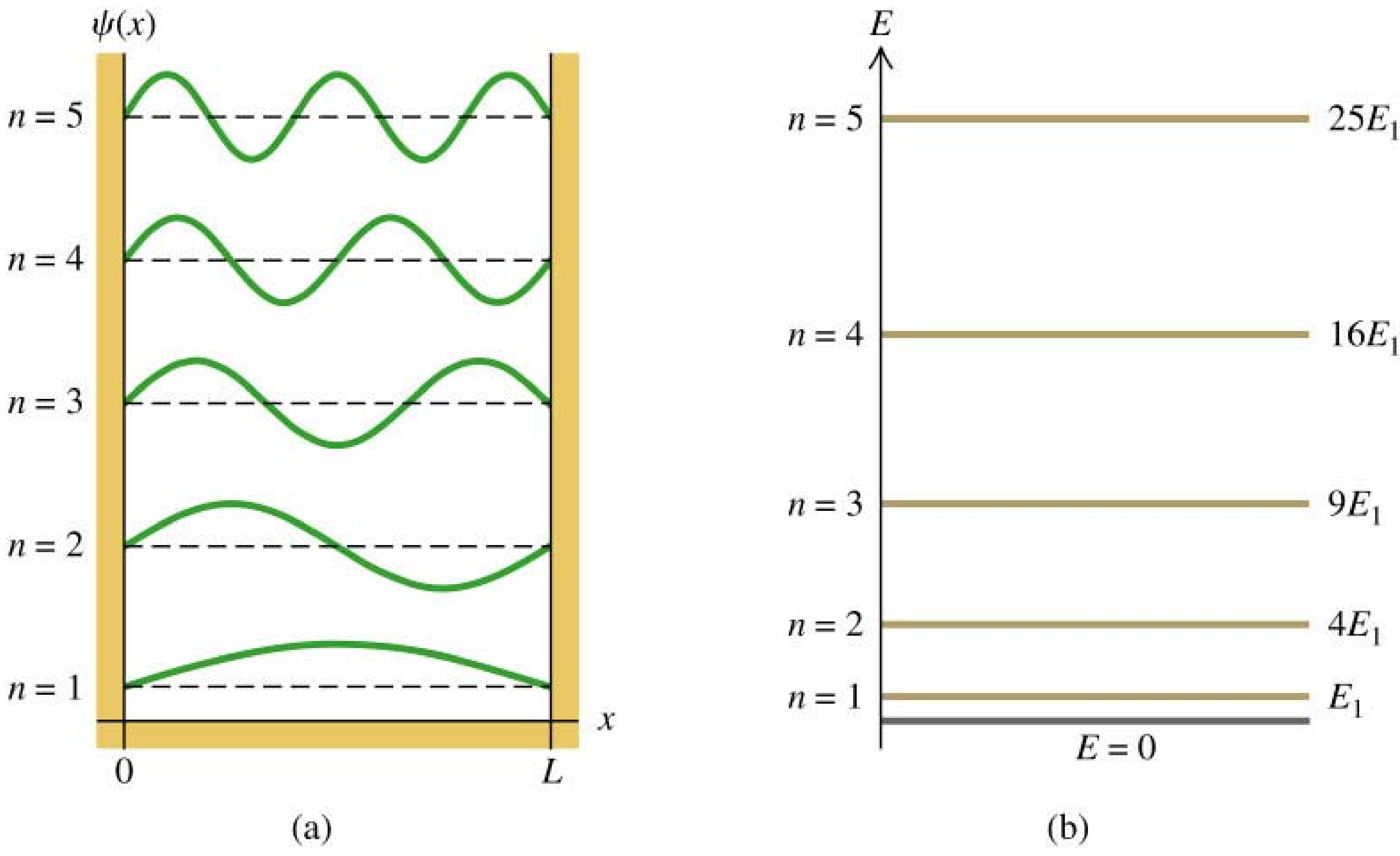
$$L = n\,\lambda_n / 2$$

Each end is a node, and there can be n-1 additional nodes in between



Wave functions for the particle in a box

$\psi(x) = 0$ --------



The energy of a particle in a box cannot be zero!

$$E_n = \frac{p_n^{\;2}}{2m} = \frac{n^2h^2}{8mL^2} = \frac{n^2\pi^2\hbar^2}{2mL^2} \qquad (n = 1, 2, 3 \ldots) \qquad (40.9)$$

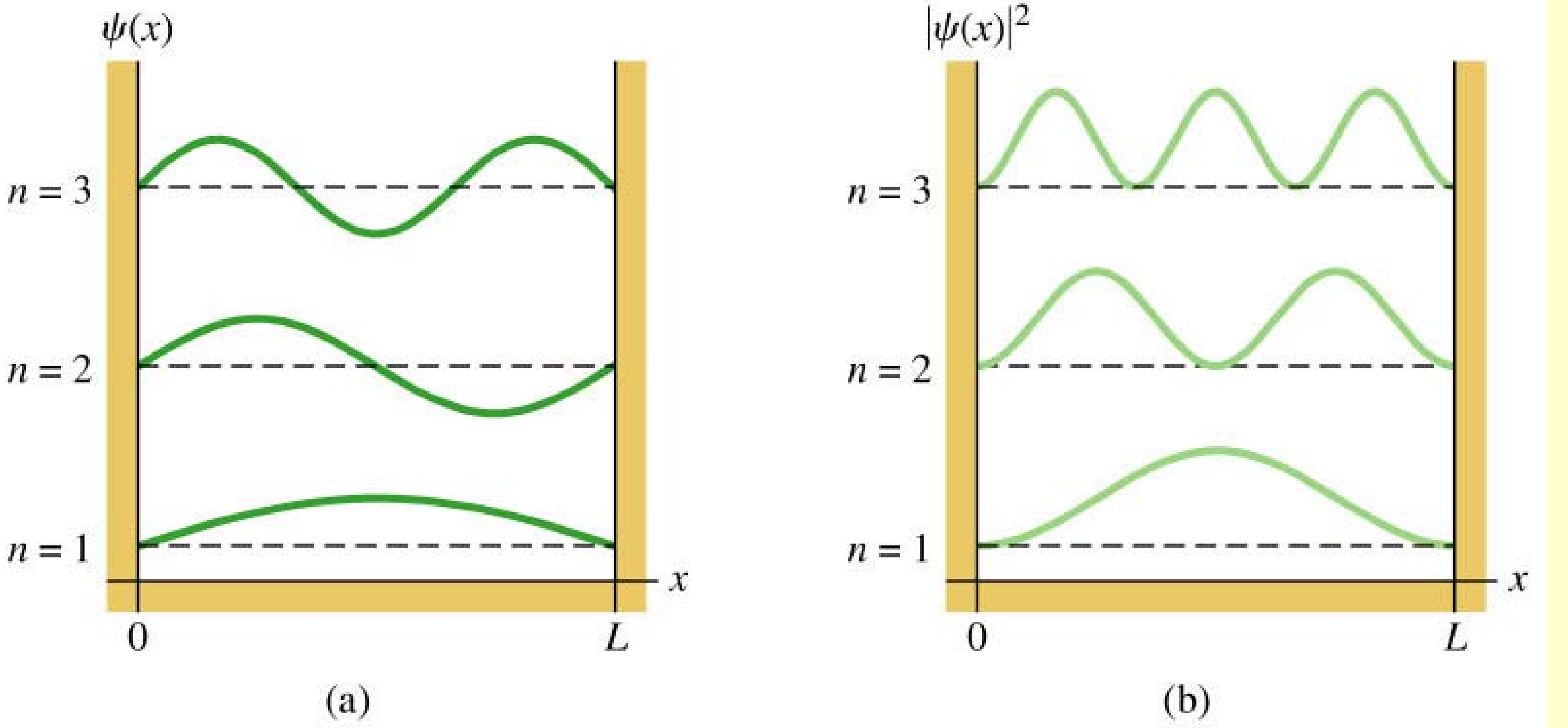
(energy levels, particle in a box)

You could try to put n = 0 into this equation, but then $\psi(x) = 0$, which would mean there is no particle!

The function $\psi(x) = C \sin(kx)$ is a solution to the Schrodinger Eq. for the particle in a box

Wave function

Probability distribution function



Q1

The first five wave functions for a particle in a box are shown. The probability of finding the particle near $x = L/2$ is

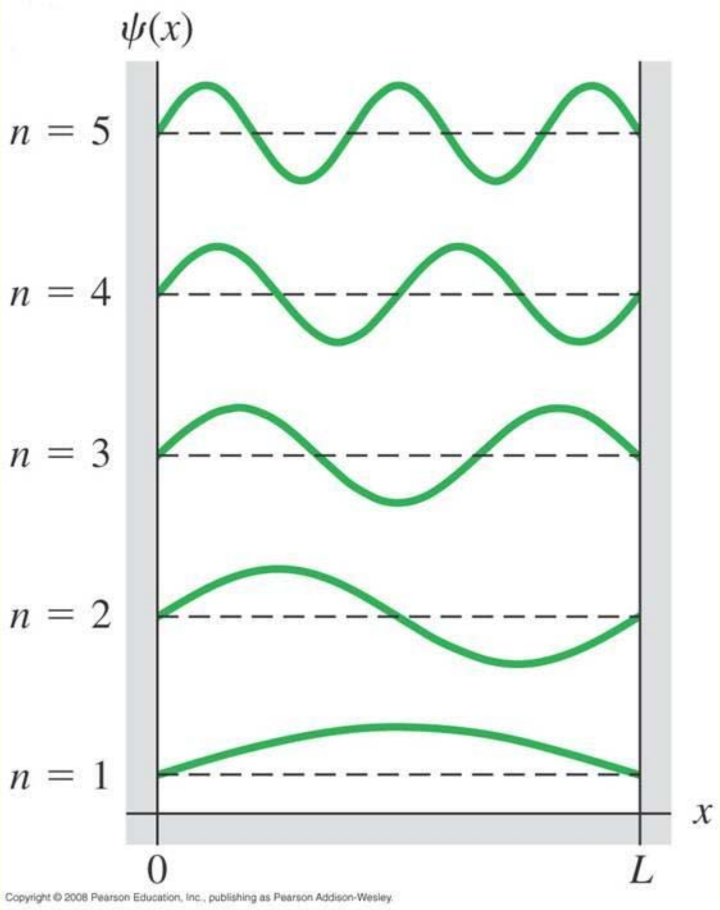
A. least for $n = 1$.

B. least for $n = 2$ and $n = 4$.

C. least for $n = 5$.

D. the same (and nonzero) for $n = 1, 2, 3, 4$, and 5.

E. zero for $n = 1, 2, 3, 4$, and 5.



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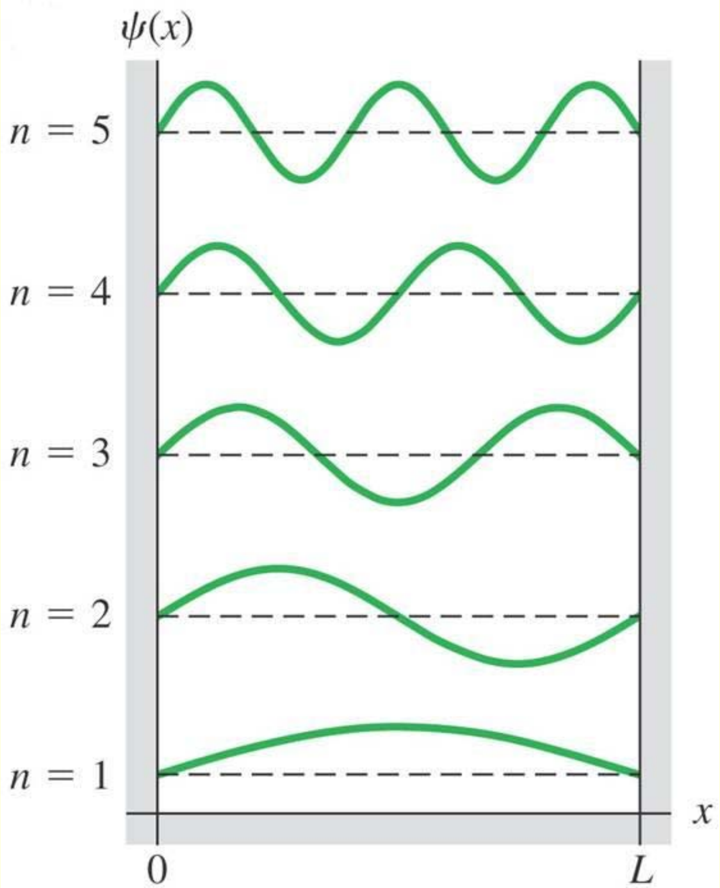


Q2

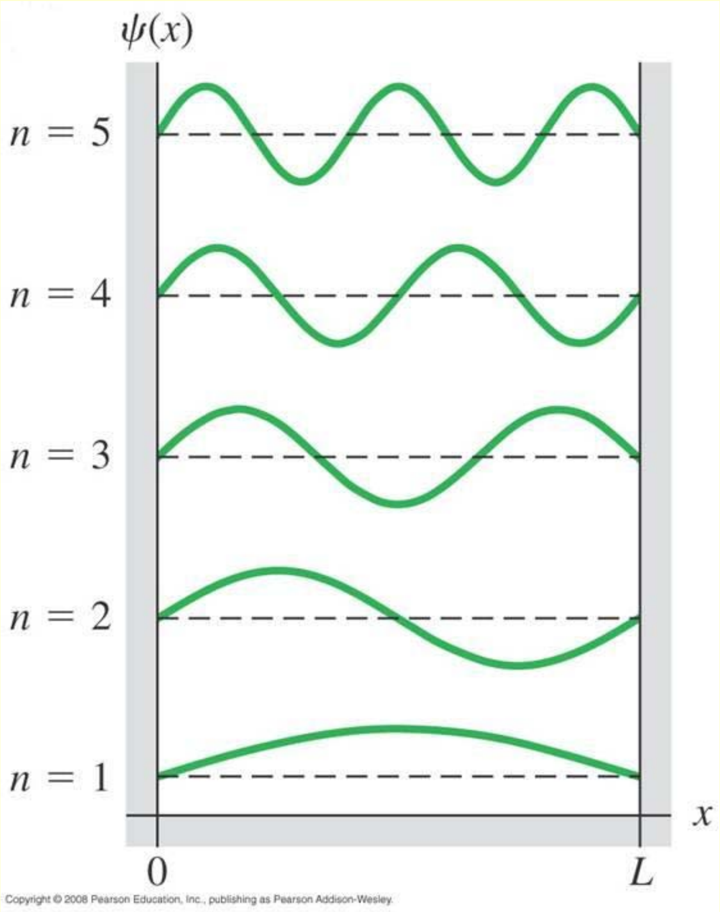
Compare n=1 and n=5 states. The average value of the *x*-component of momentum is

A. least for *n* = 1.

B. least for *n* = 5.

C. the same (and nonzero) for *n* = 1 and *n* = 5.

D. zero for both *n* = 1 and *n* = 5.



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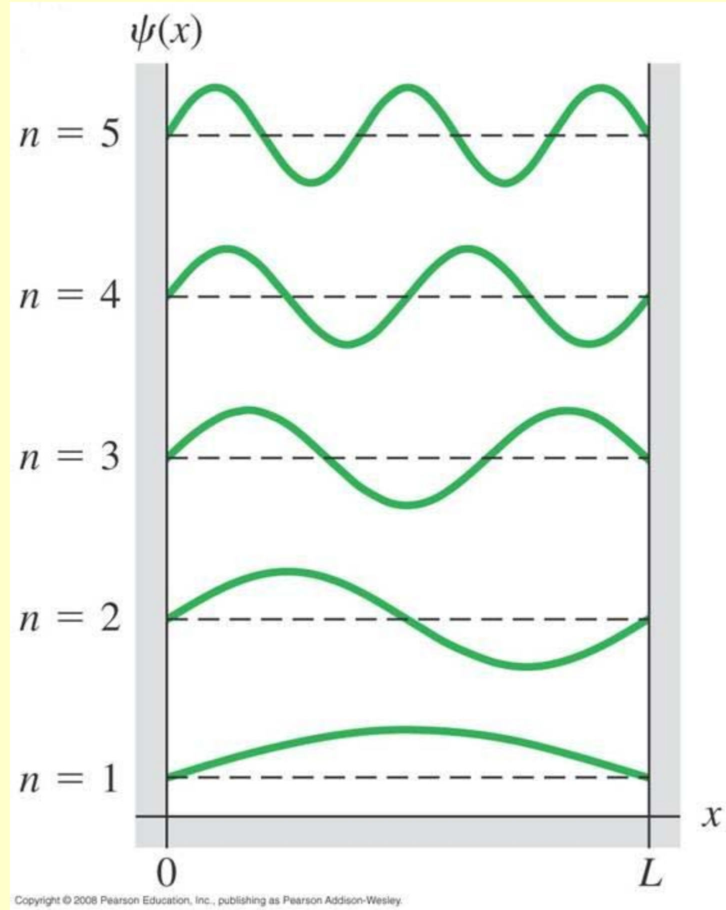


A. least for $n = 1$.

B. least for $n = 5$.

C. the same (and nonzero) for $n = 1$ and $n = 5$.

D. zero for both $n = 1$ and $n = 5$.

The wave functions for the particle in a box are superpositions of waves propagating in opposite directions. One wave has p_x in one direction, the other has p_x in the other direction, averaging to zero.

Q3

The first five wave functions for a particle in a box are shown. Compared to the n = 1 wave function, the n = 5 wave function has

$$E_n = \frac{p_n^{\ 2}}{2m} = \frac{n^2 h^2}{8mL^2} = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

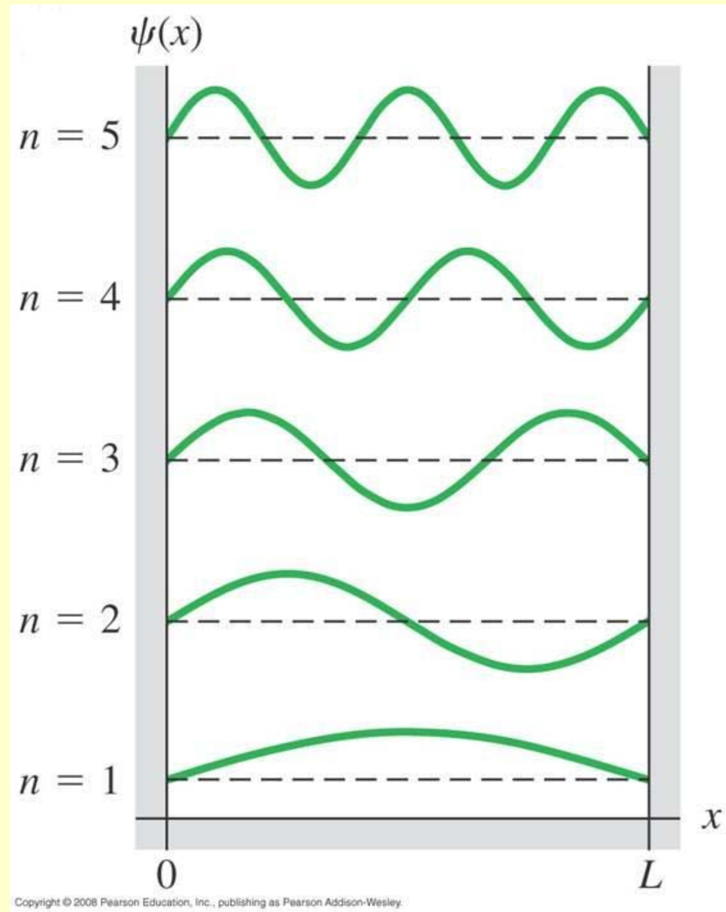
A. the same kinetic energy (KE).

B. 5 times more KE.

C. 25 times more KE.

D. 125 times more KE.

E. none of the above



A3

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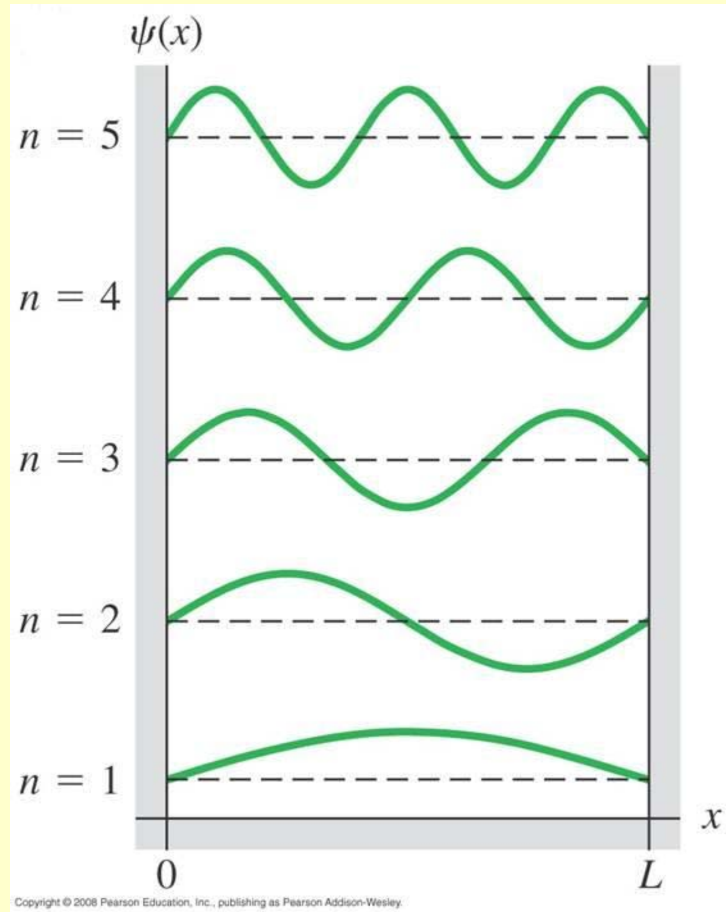

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B. 5 times more KE.

C. 25 times more KE.

D. 125 times more KE.

E. none of the above

Normalization

Not every function has this property:

$$\int_{-\infty}^{\infty} |\psi(x)|^2\, dx = 1 \qquad \text{(normalization condition)} \qquad (40.11)$$

If a function $\psi(x)$ has this property, it is "normalized".

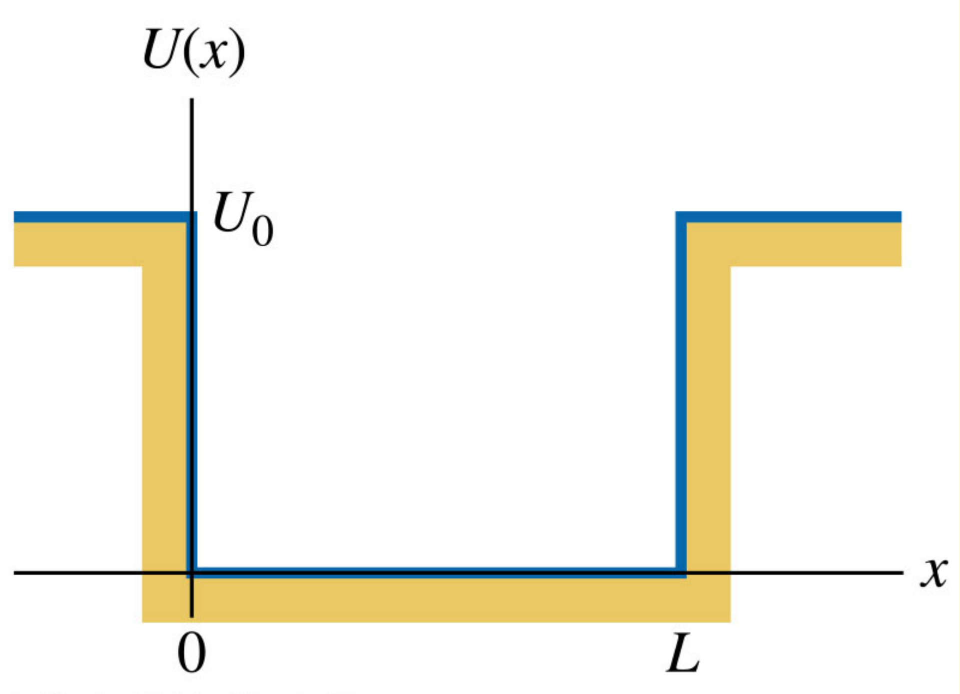
You can find C so that the function $\psi(x) = C \sin(n\pi x/L)$ is normalized.

$$C = \sqrt{\frac{2}{L}}$$

Particle in a square well

Example: electron in a metallic sheet of thickness L, moving perpendicular to the surface of the sheet

U_0 is related to the work function.

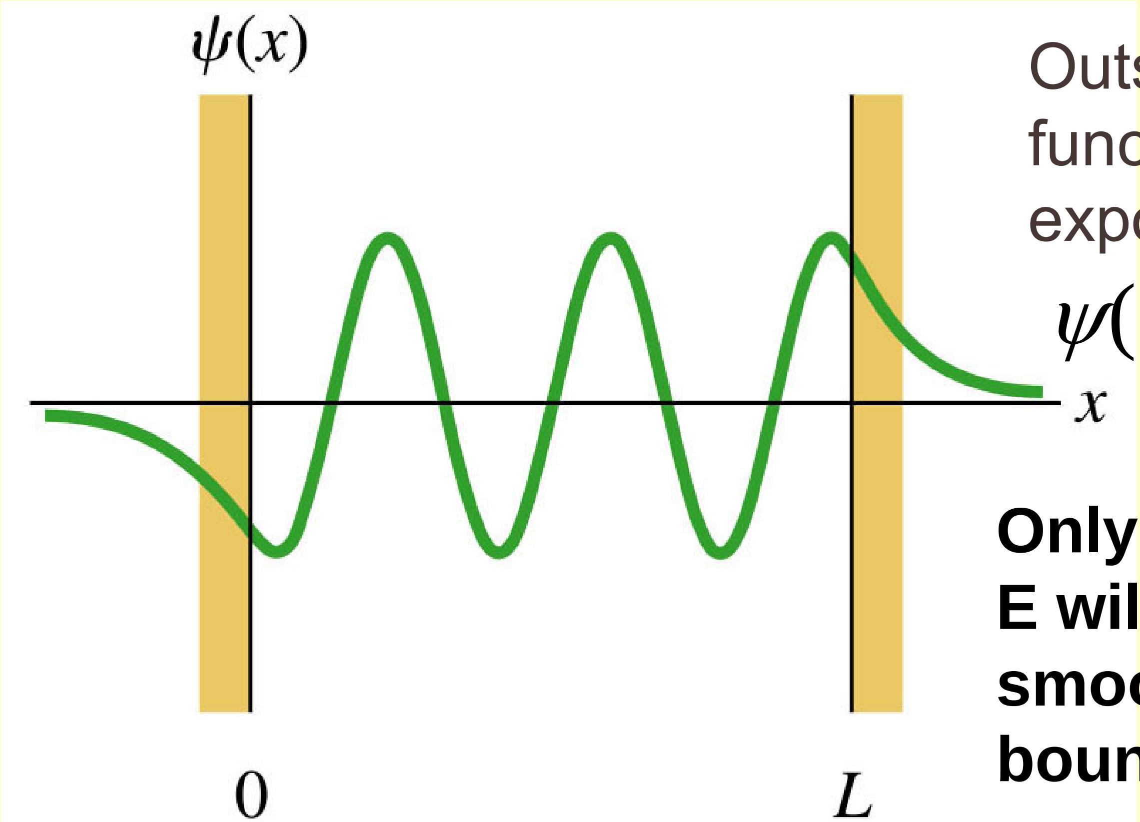


Newton: particle is trapped unless $E > U_0$

QM: For $E < U_0$, the particle is "bound"

Inside the well (0<x<L), the solution to the SE is similar to the particle in the box (sinusoidal)

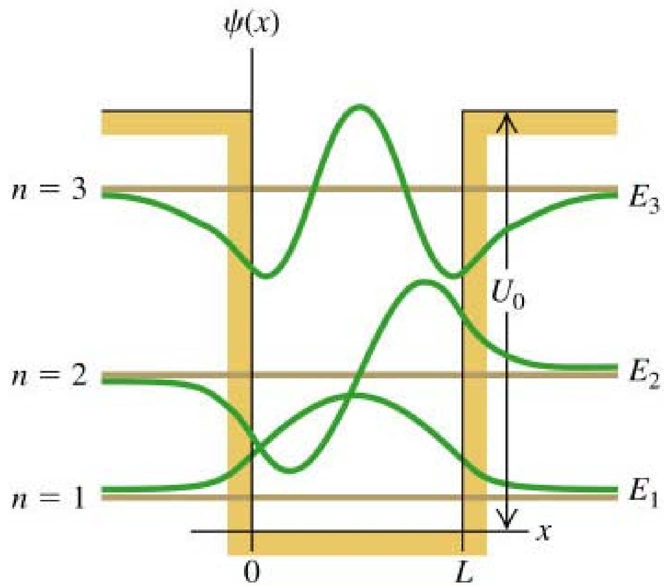
$$\psi(x) = A\cos\frac{\sqrt{2mE}}{\hbar}x + B\sin\frac{\sqrt{2mE}}{\hbar}x$$

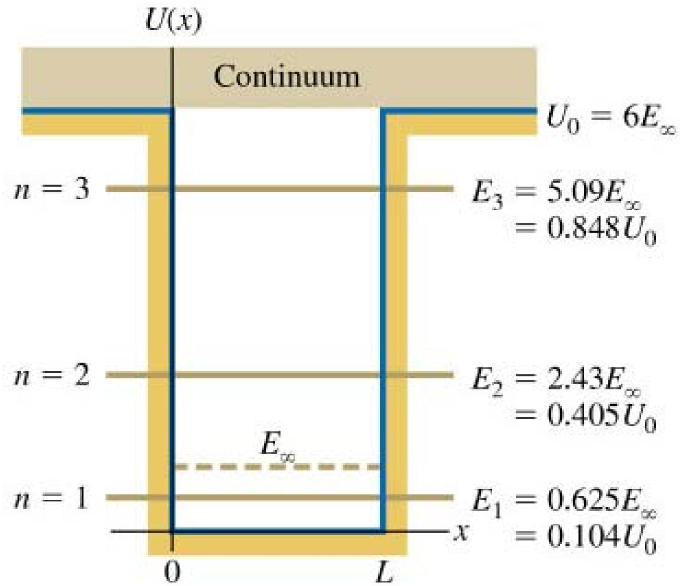


Outside, the wave function decays exponentially:

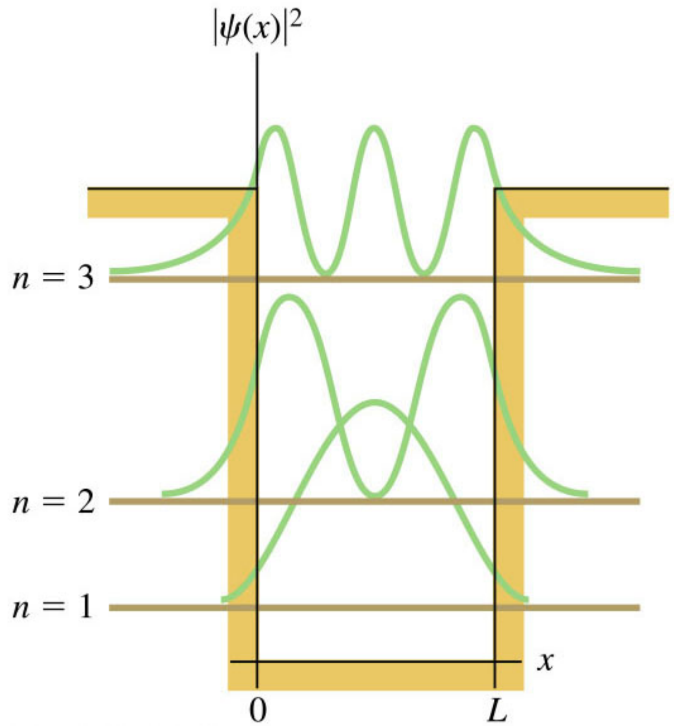
$$\psi(x) = Ce^{\kappa x} + De^{-\kappa x}$$

Only for certain values of E will these functions join smoothly at the boundaries!





(b)



Non-zero probability of
it being outside the
well!
Forbidden by
Newtonian mechanics.

This leads to some very odd behavior… quantum tunneling!

Q4

The first three wave functions for a finite square well are shown. The probability of finding the particle at $x > L$ is

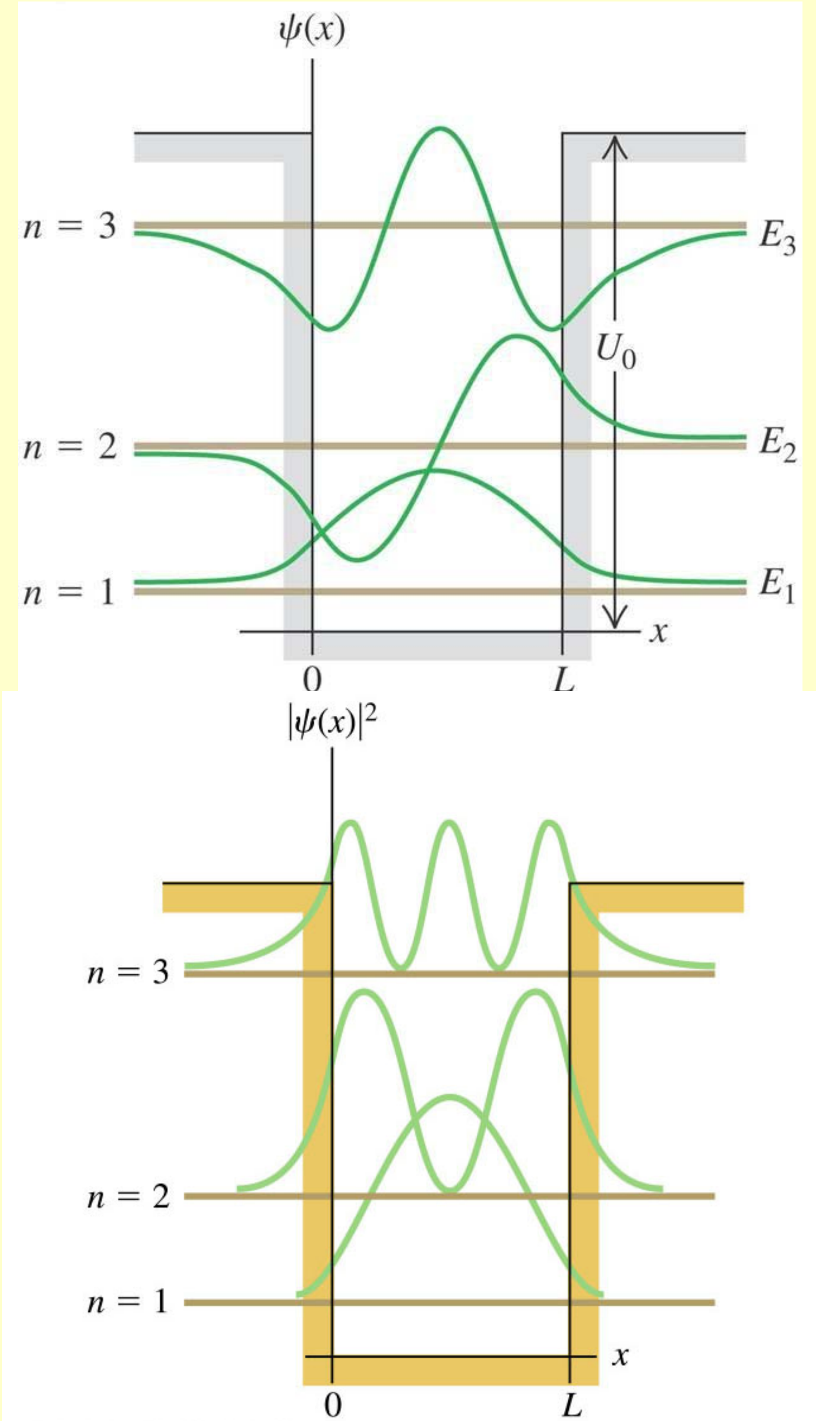
A. least for $n = 1$.

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.



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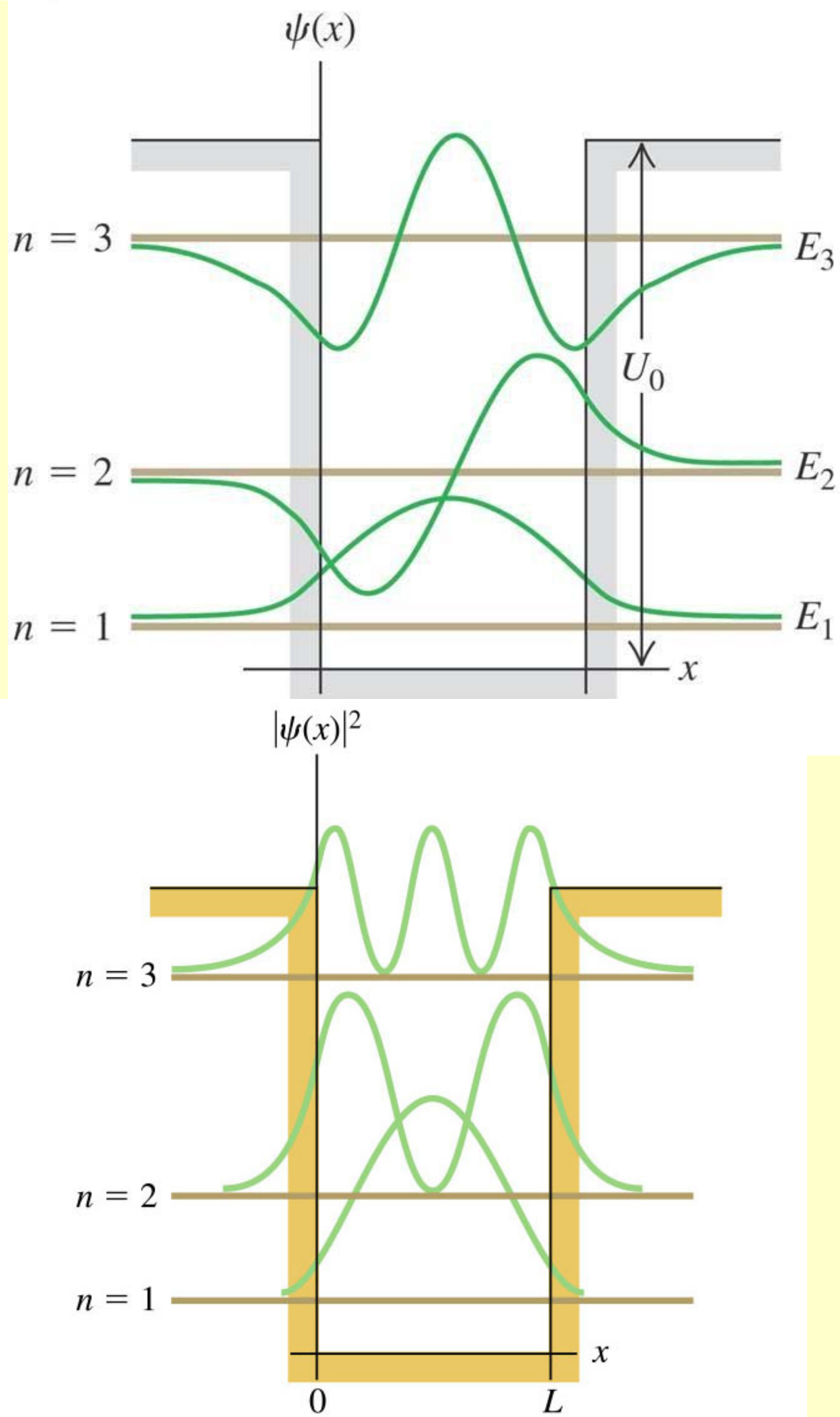
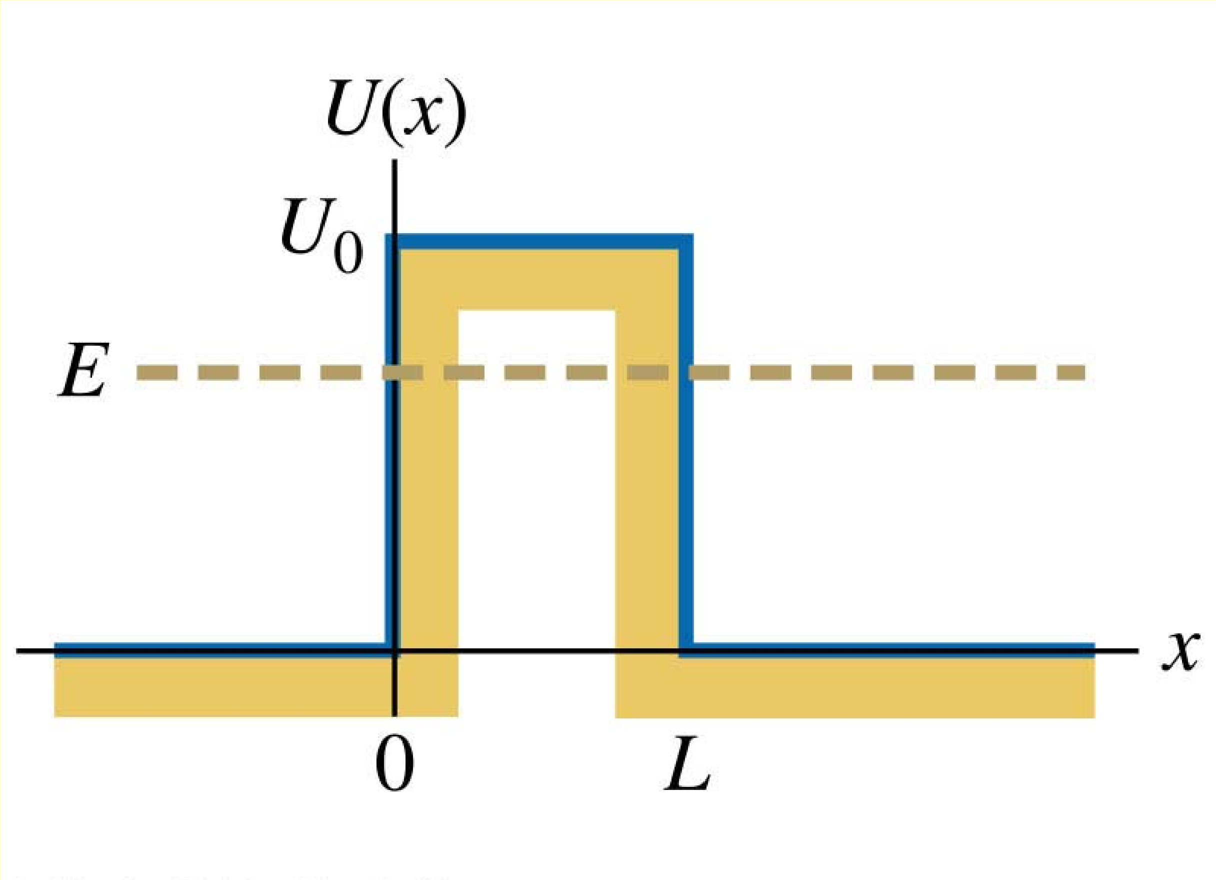


Potential barriers and quantum tunneling

- **Non-zero probability that a particle can "tunnel" through a barrier!**
- **No concept of this from classical physics.**



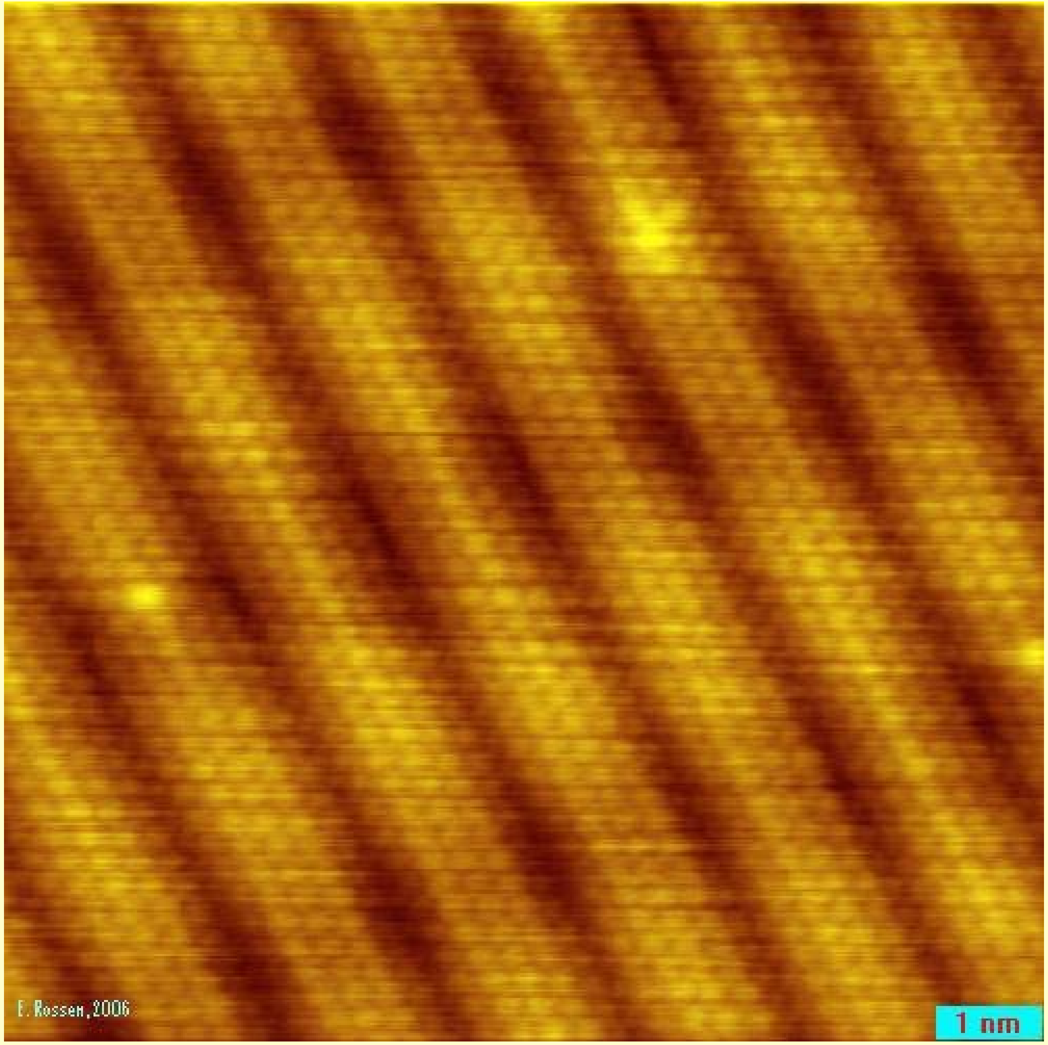
Potential barriers and quantum tunneling

Importance:

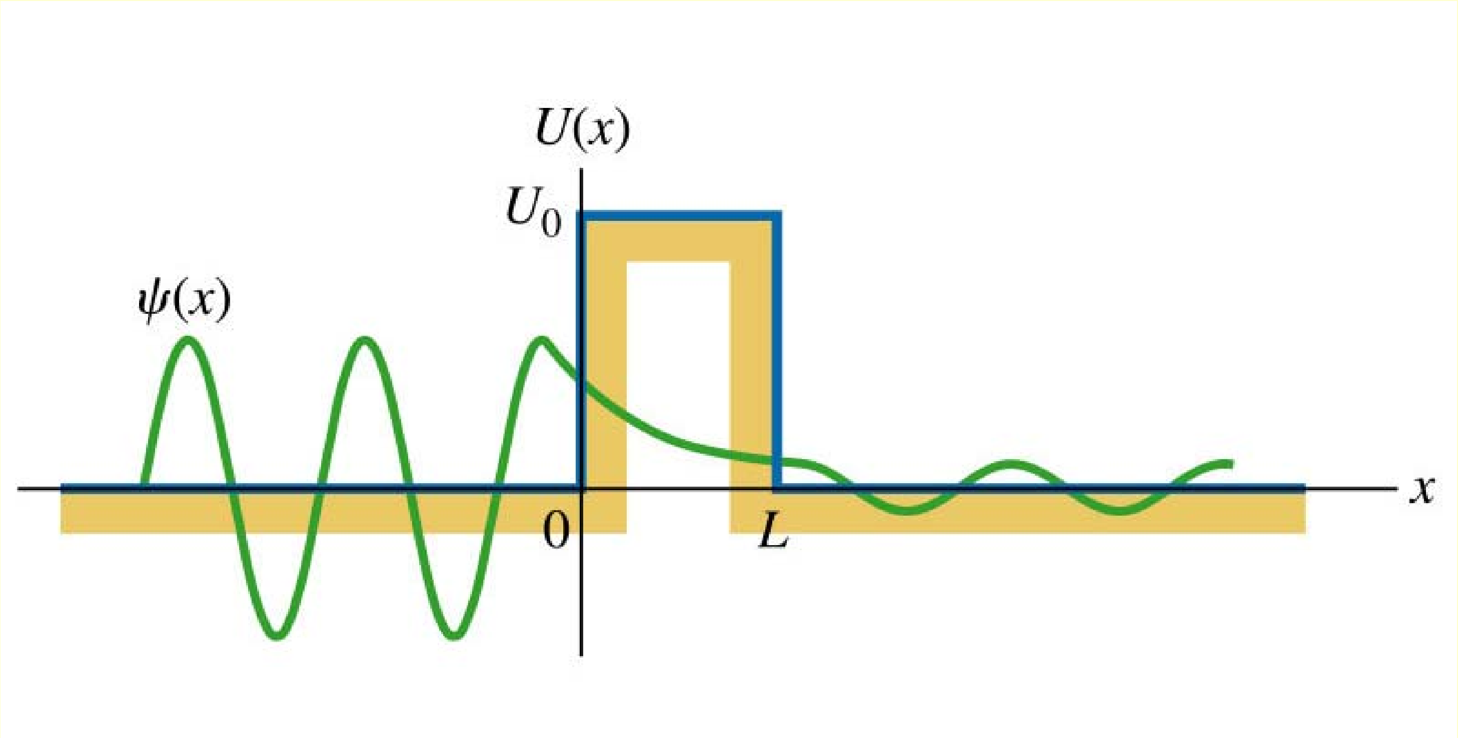
- Tunnel diode in a semiconductor: Current is switched on/off ~ps by varying the height of the barrier
- Josephson junction: e- pairs in superconductors can tunnel through a barrier layer: precise voltage measurements; measure very small B fields.
- Scanning tunneling microscope (STM): view surfaces at the atomic level!
- Nuclear fusion
- Radioactive decay

Scanning tunneling microscope (~atomic force microscope)

Au(100) surface : STM resolves individual atoms!

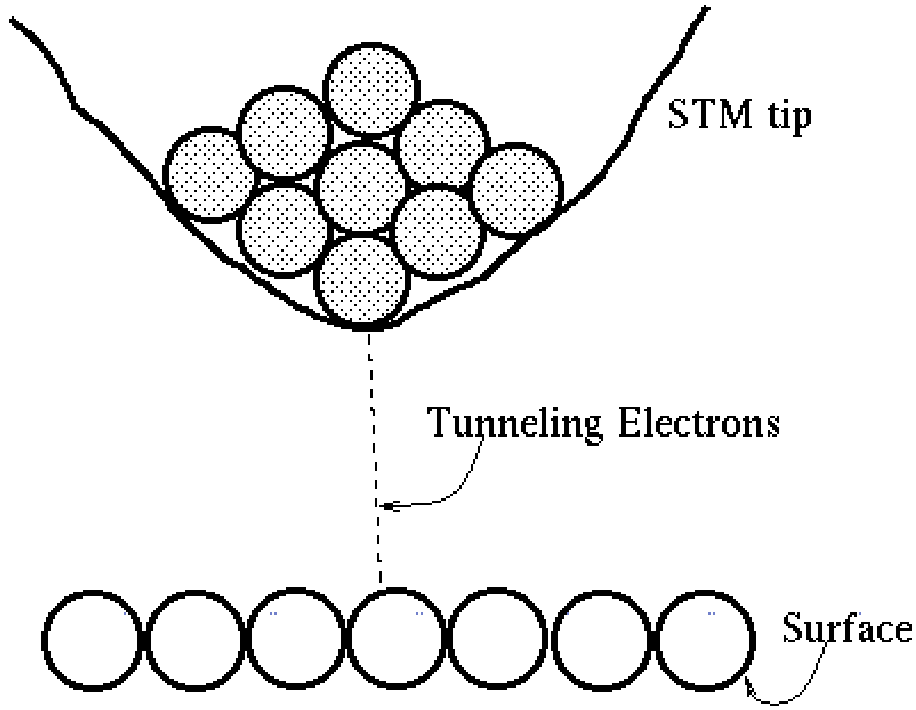


A wave function for a particle tunneling through a barrier

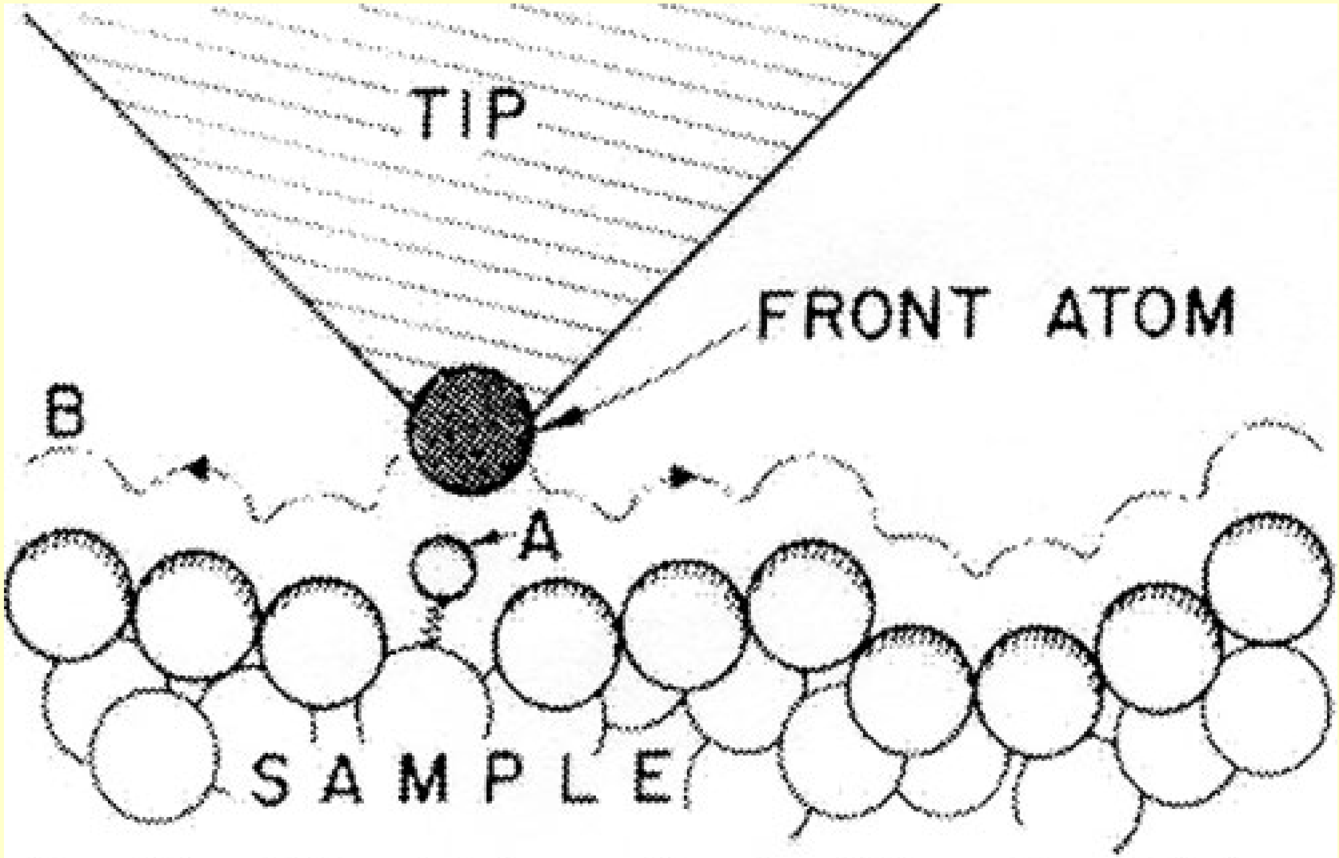


$\psi(x)$ and $d\psi/dx$ must be continuous at 0 and L.

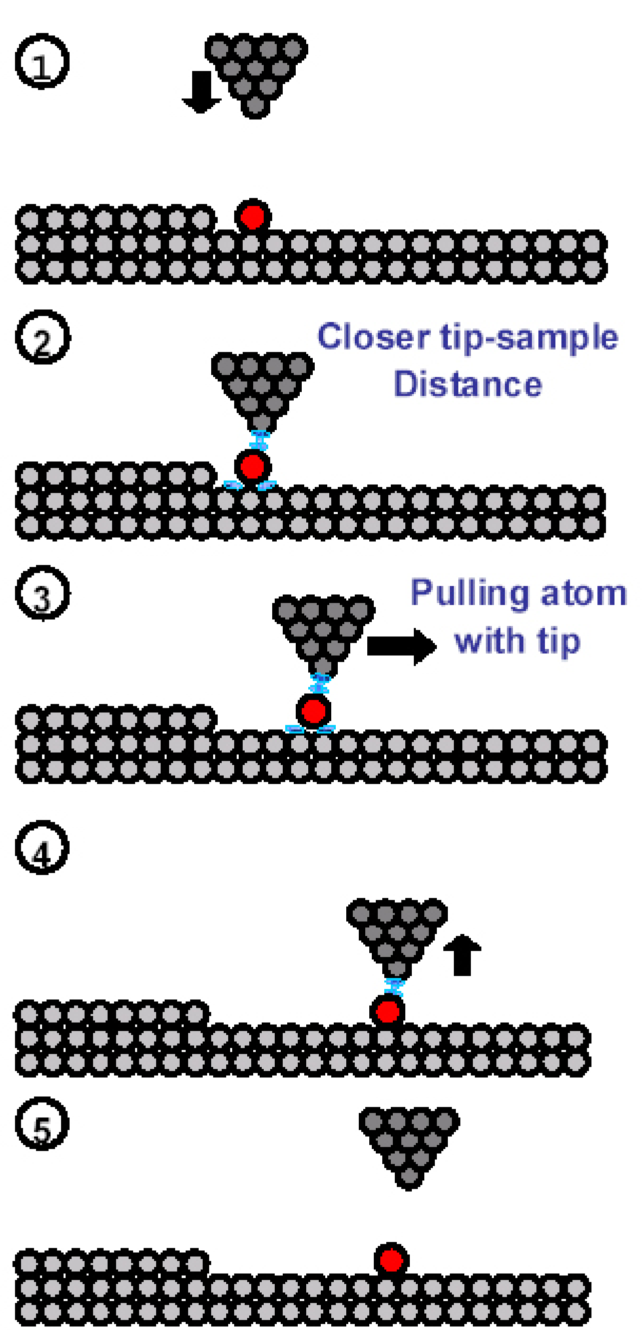
The Scanning Tunneling Microscope



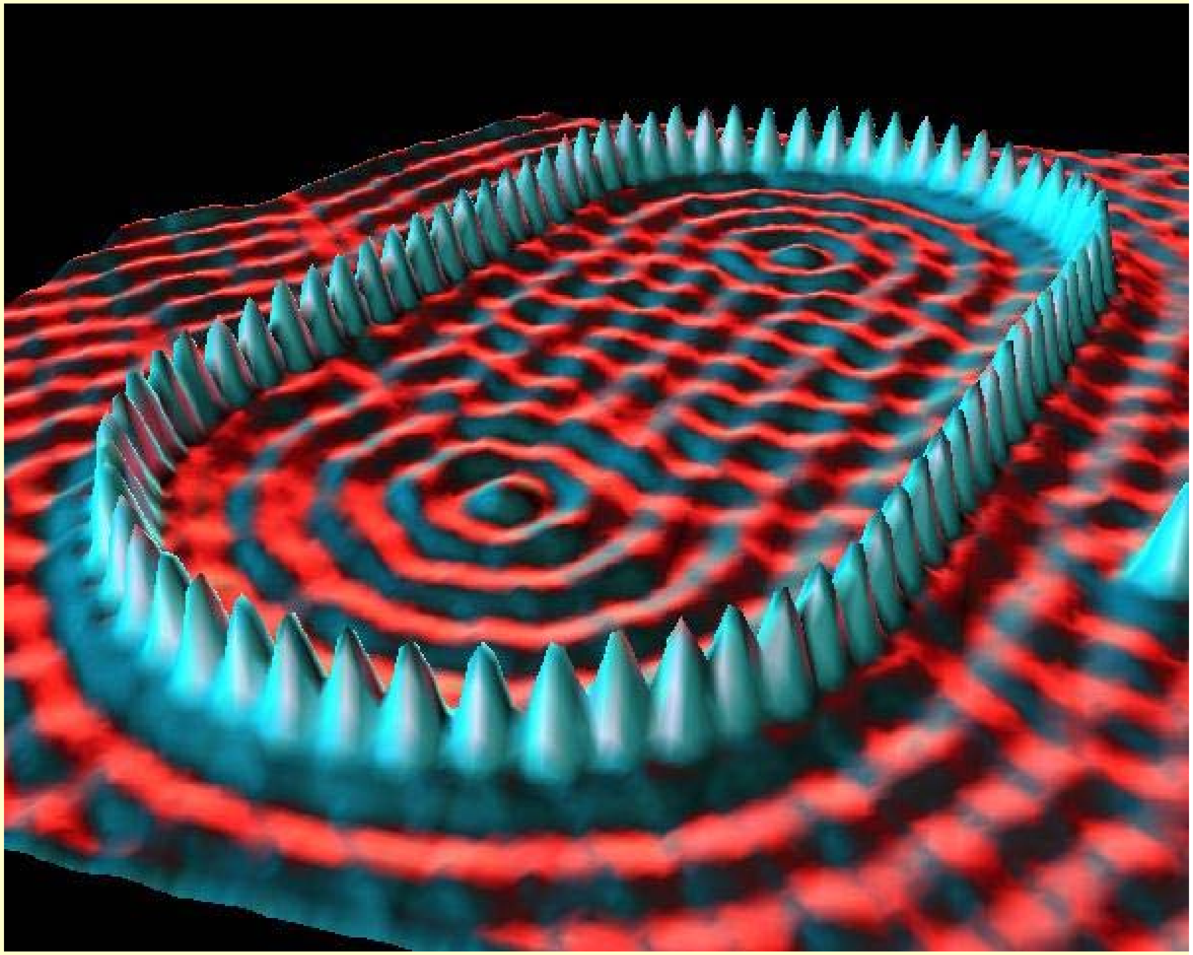
The Scanning Tunneling Microscope (STM) was developed by Gerd Binnig and Heinrich Rohrer at IBM. When a metal tip is brought near a conducting surface, electrons can tunnel from the tip to the surface or vice–versa. Because the tunneling probability is exponentially dependent on the distance the contours of the surface can be mapped out by keeping the current constant and measuring the height of the tip. In this way, atomic resolution can be obtained. For their work, Binnig and Rohrer shared the 1986 Nobel Prize.



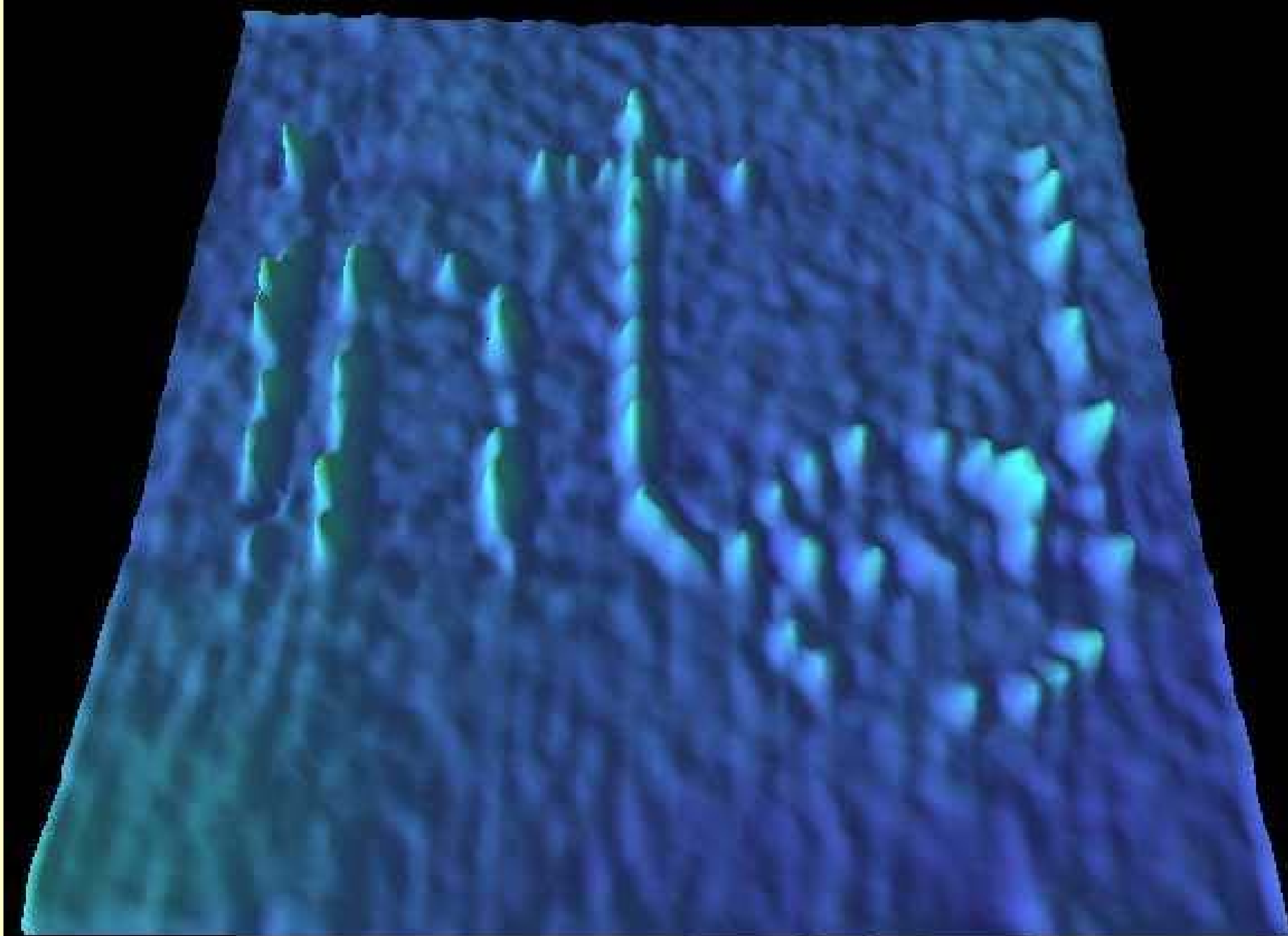
Description of the principle operation of an STM as well as that of an AFM.
The tip follows contour B, in one case to keep the tunneling current constant (STM) and in the other to maintain constant force between tip and sample (AFM, sample, and tip either insulating or conducting). The STM itself may probe forces when a periodic force on the adatom A varies its position in the gap and modulates the tunneling current in the STM. The force can come from an ac voltage on the tip, or from an externally applied magnetic field for adatoms with a magnetic moment.



Scanning tunneling microscope (STM)

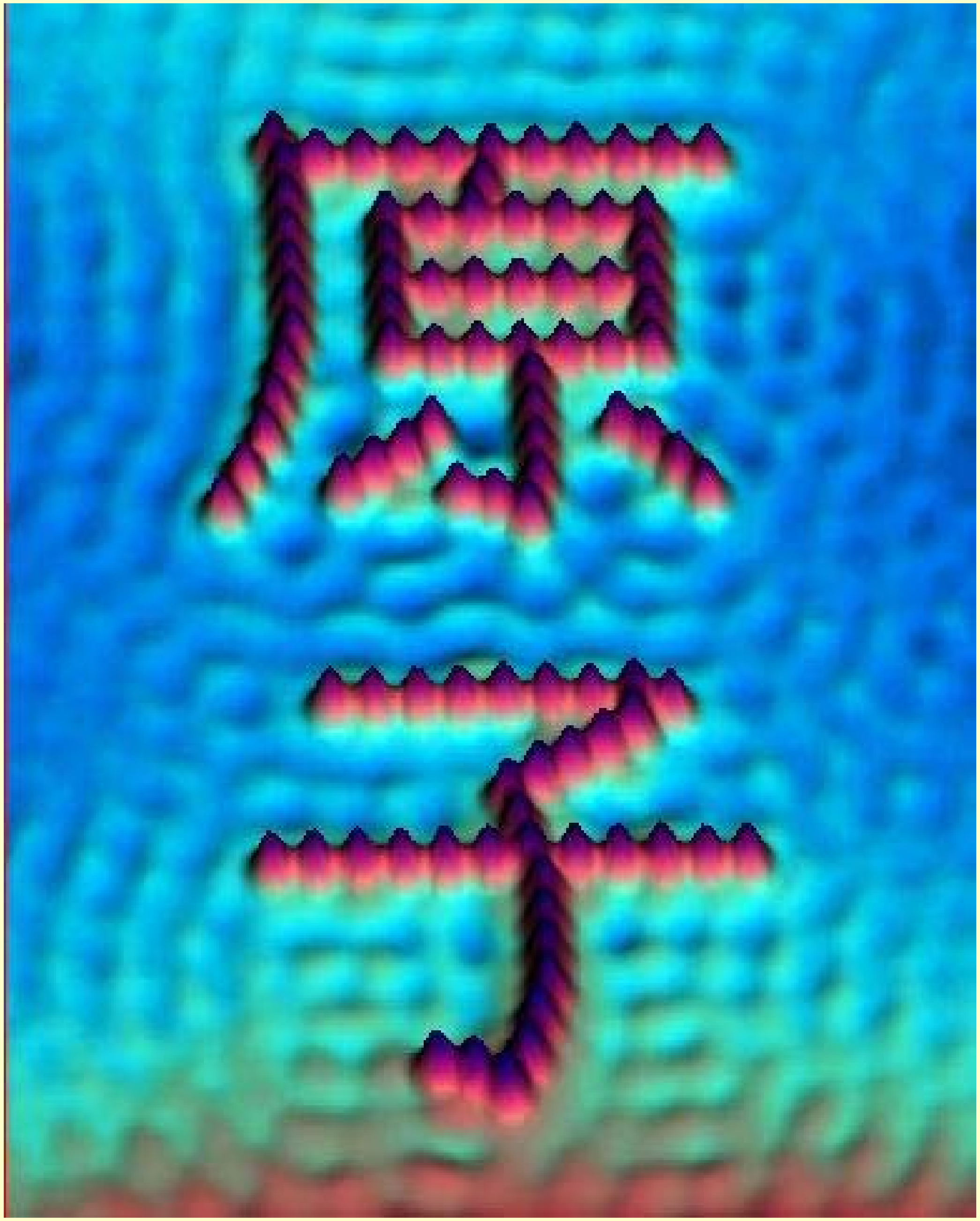


Iron atoms can be arranged to make an “electron corral” (IBM’s Almaden Research Center)



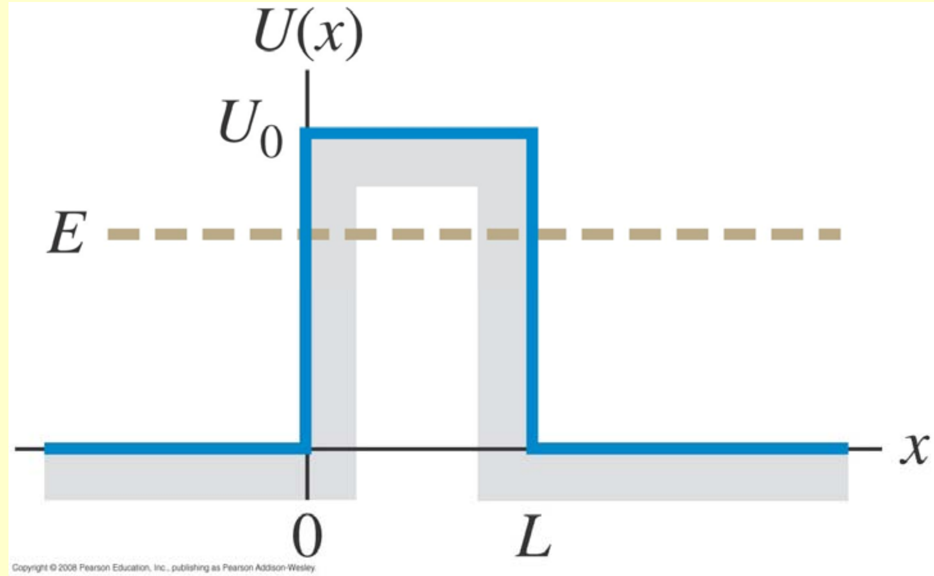
500 nm x 500 nm

Iron on copper(111)



Q5

A potential-energy function is shown. If a quantum-mechanical particle has energy $E < U_0$, the particle has zero probability of being in the region



A. $x < 0$.

B. $0 < x < L$.

C. $x > L$.

D. the particle can be found at any x

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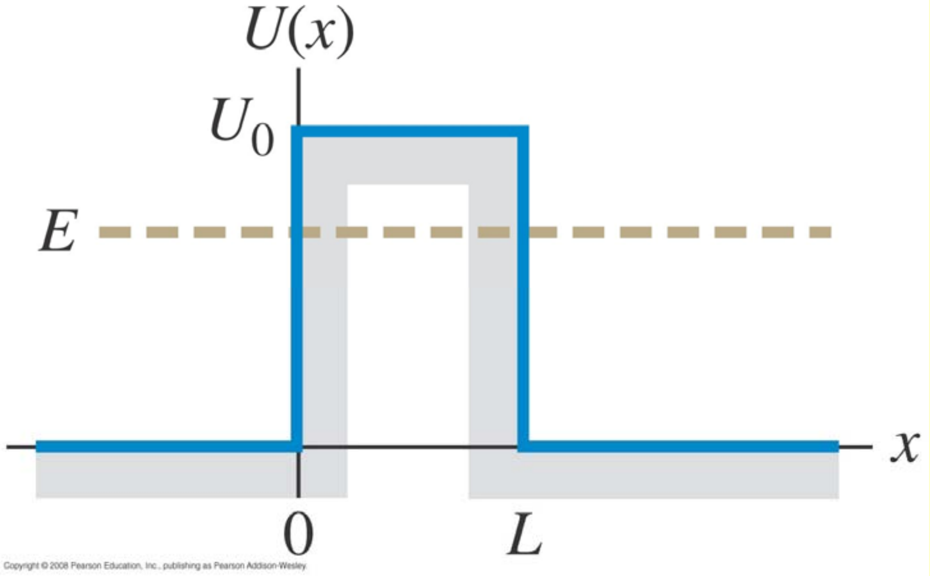

A. $x < 0$.

B. $0 < x < L$.

C. $x > L$.

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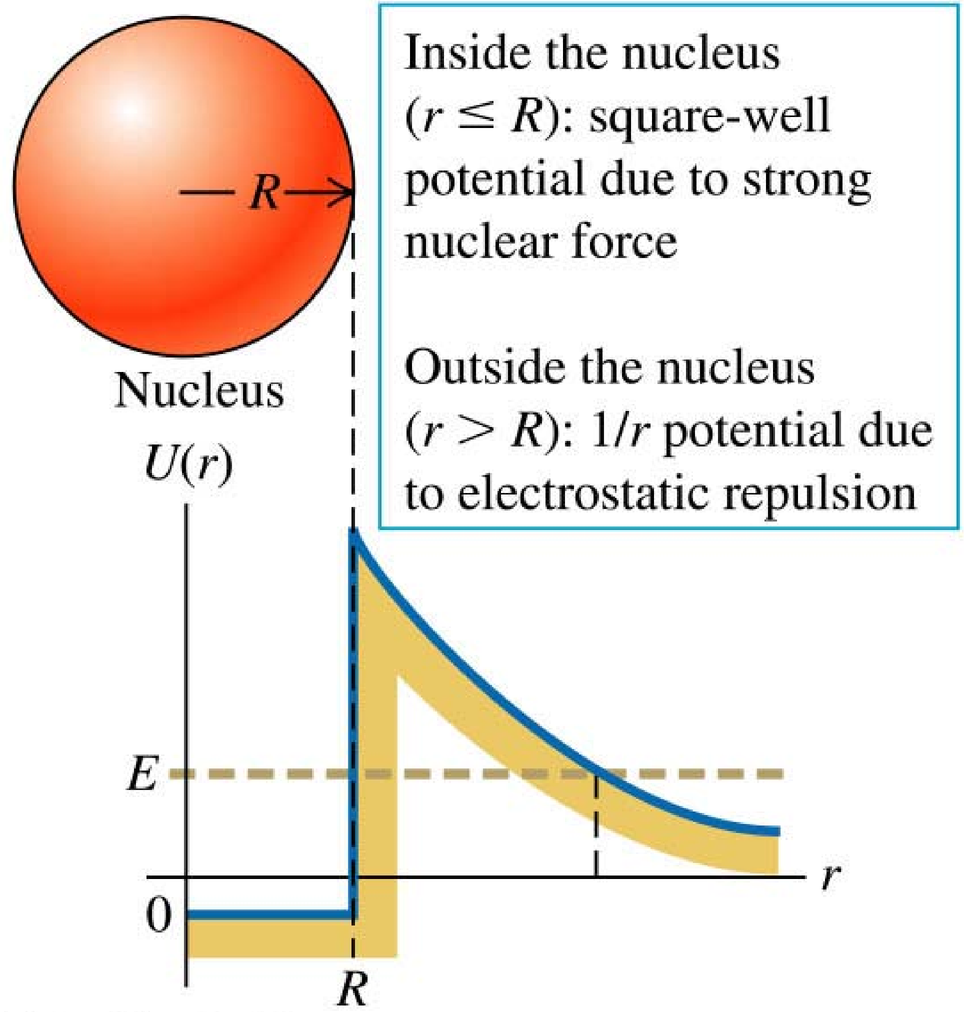
An alpha particle in a nucleus.
If E > 0, it can tunnel through the barrier and escape from the nucleus.

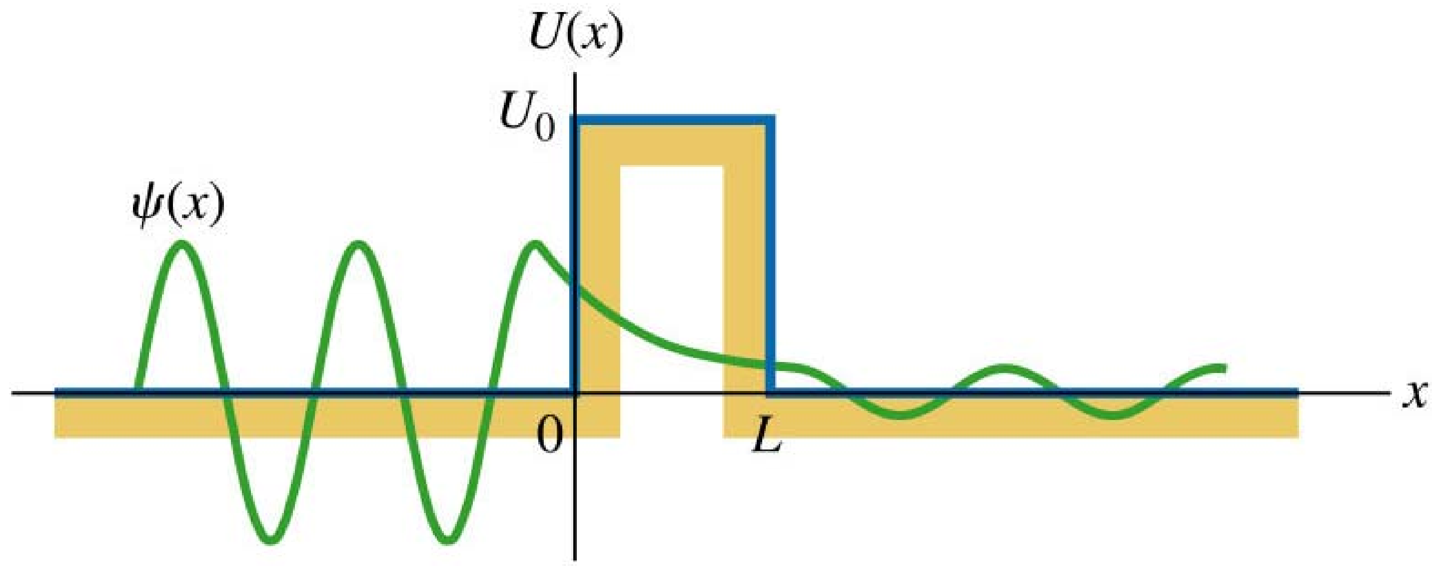


Approx. probability of tunneling (T<<1):

$$T = Ge^{-2\kappa L}$$

where $$G = 16\frac{E}{U_0}\left(1 - \frac{E}{U_0}\right)$$

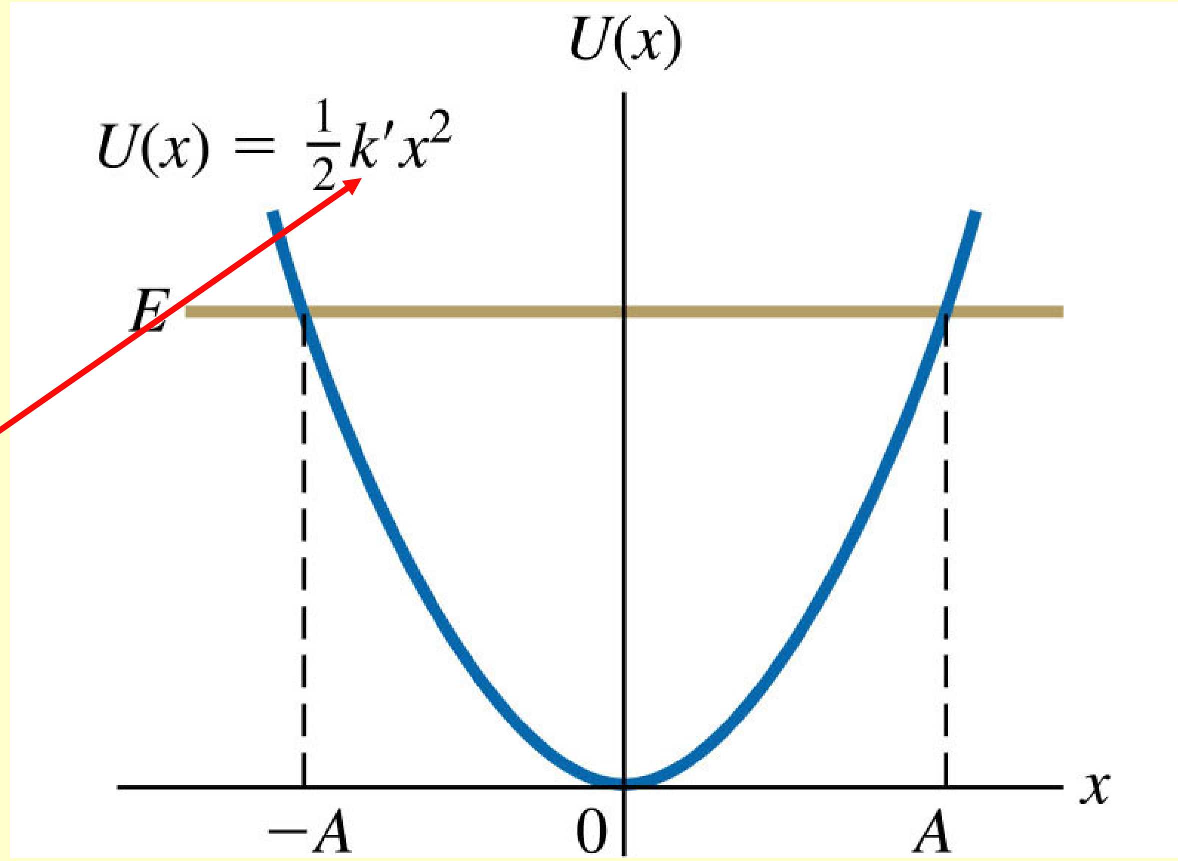
$$\kappa = \frac{\sqrt{2m(U_0 - E)}}{\hbar}$$



The quantum harmonic oscillator

$$\omega = \sqrt{\frac{k_{spring}}{m}}$$

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



The Schrodinger equation for the harmonic oscillator

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}k_{spring}x^2\psi=E\psi$$

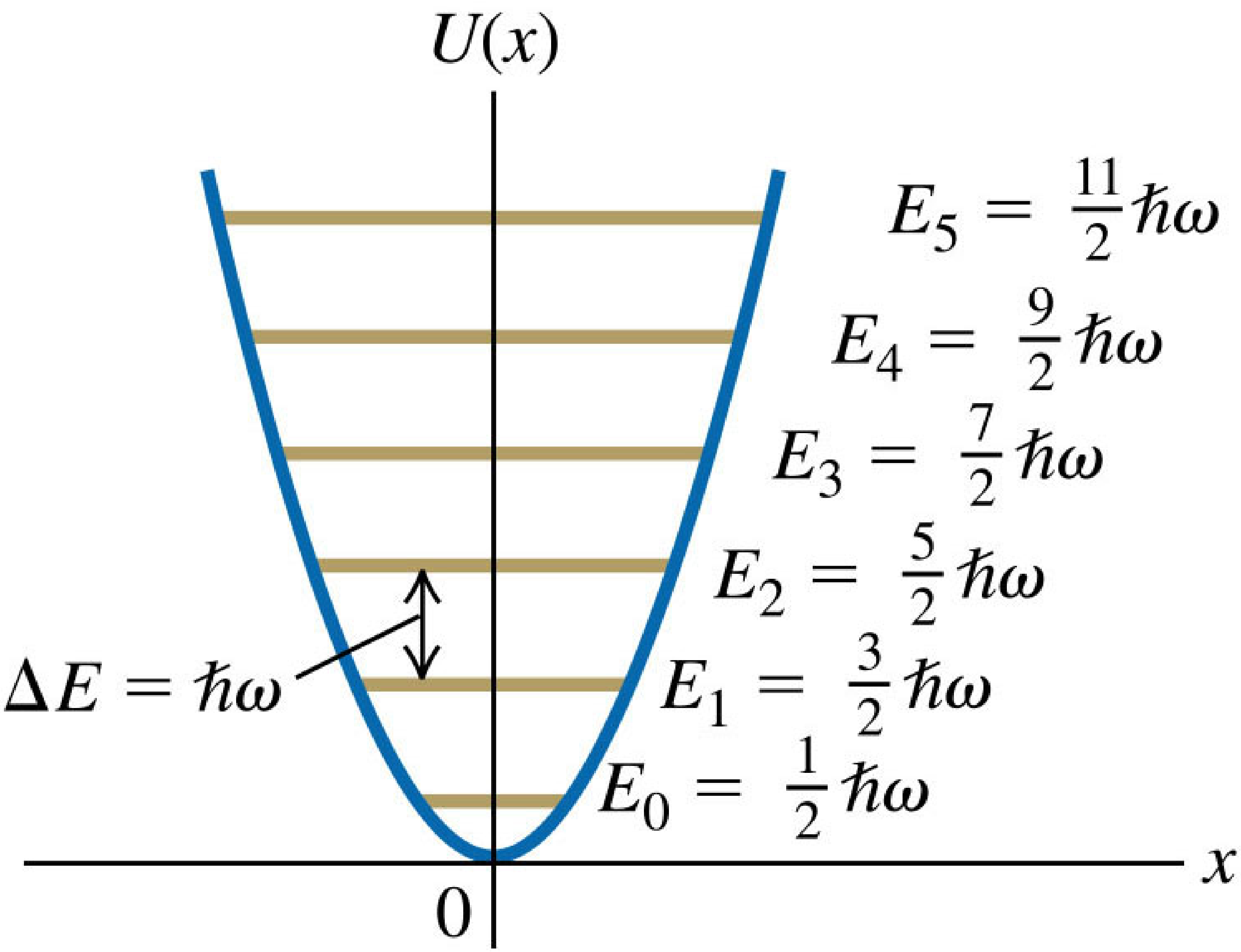
The solution to the SE is

$$\psi(x)=Ce^{-\sqrt{mk_{spring}}x^2/2\hbar}$$

Solving for E gives the energy

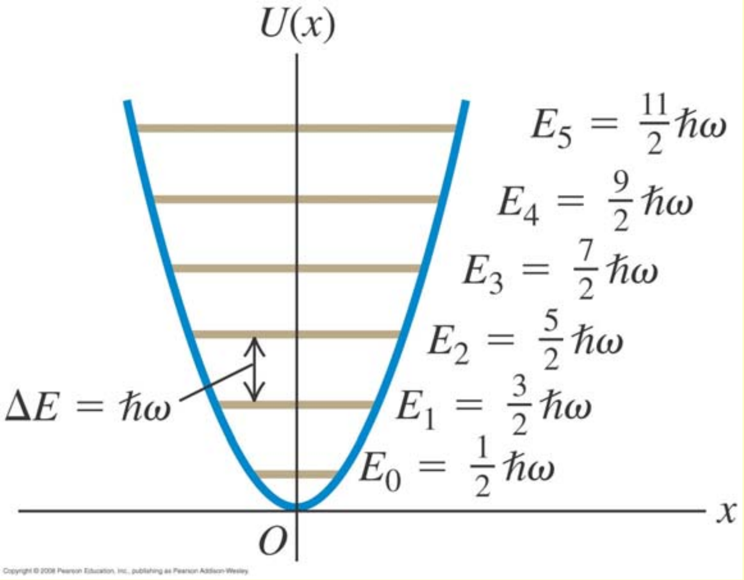
$$E_n = \left(n + \frac{1}{2}\right)\hbar\sqrt{\frac{k'}{m}} = \left(n + \frac{1}{2}\right)\hbar\omega \qquad (n = 0, 1, 2, \ldots) \qquad (40.26)$$

(energy levels, harmonic oscillator)



Q6

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.

A6

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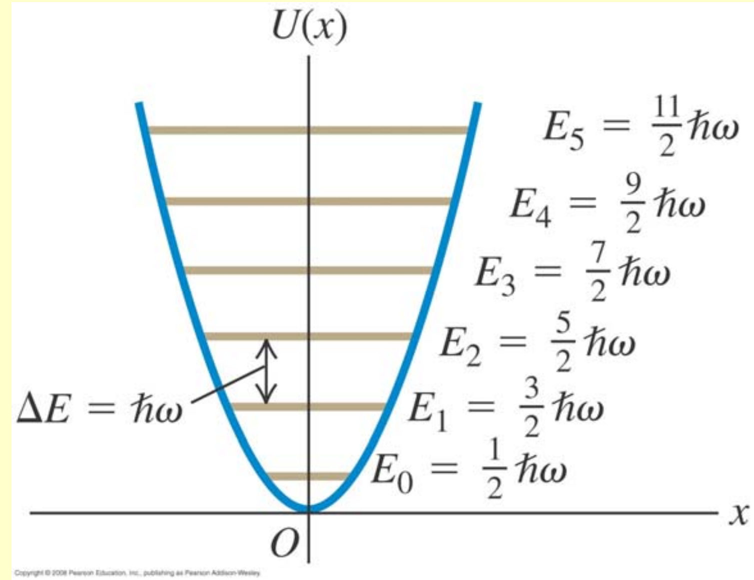

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