PEN205
MODERN PHYSICS

Quantum Mechanics – II

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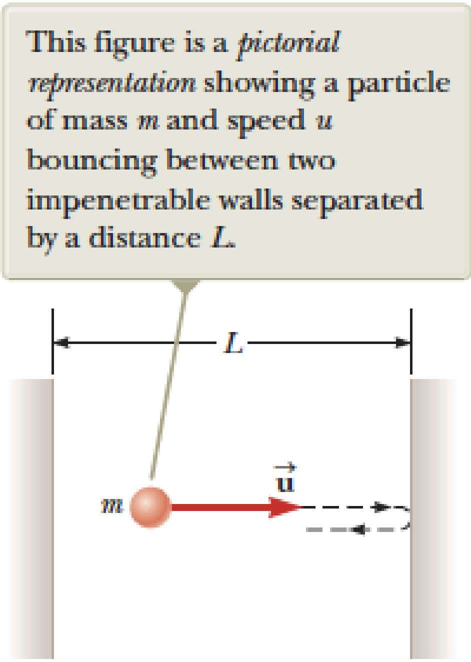
Quantum Particle Under Boundary Conditions

In this section, we will investigate the effects of restrictions on the motion of a quantum particle

A Particle in a Box

A particle confined to a one-dimensional region of space, called the *particle-in-a-box* problem

from a classical viewpoint;



its momentum ($m\mathbf{u}$) and kinetic energy remains constant

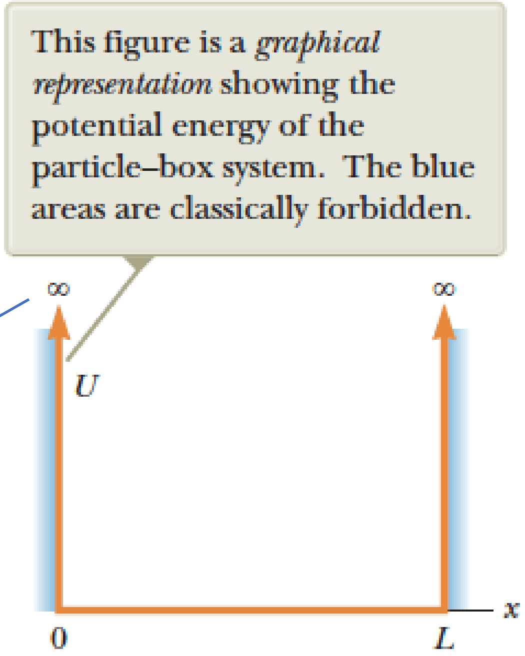
quantum-mechanical approach;

Because the walls are impenetrable → $\psi(x)$ must be zero for $x < 0$ and $x > L$

Also, $\boldsymbol{\psi}$ must also be zero at the walls → $\psi(0) = 0 \qquad \psi(L) = 0$

Only those wave functions that satisfy these boundary conditions are allowed

As long as the particle is inside the box, the potential energy of the system does not depend on the location of the particle and we can choose its constant value to be zero.



∞ → the only way a particle could be outside the box is if the system has an infinite amount of energy, which is impossible!

The wave function for a particle in the box can be expressed as a real sinusoidal function: $\psi(x) = A \sin\left(\frac{2\pi x}{\lambda}\right)$

de Broglie wavelength of particle (λ)

Let's see the boundary conditions ;

→ The boundary condition **ψ**(0) = 0 is satisfied already because the sine function is zero when x = 0.

→ **ψ**(L) = 0 gives; $\psi(L) = 0 = A \sin\left(\frac{2\pi L}{\lambda}\right)$ → This is satisfied if: $\frac{2\pi L}{\lambda} = n\pi \rightarrow \lambda = \frac{2L}{n} \quad n = 1, 2, 3, \ldots$

only certain wavelengths for the particle are allowed!

Each of the allowed wavelengths corresponds to a <u>quantum state</u> for the system, and <u>n is the quantum number</u>

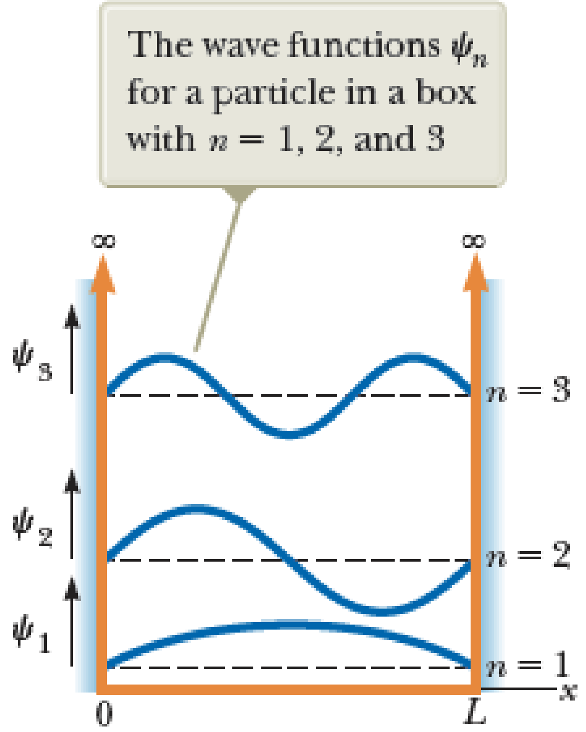
Wave functions for a particle in a box: $\psi_n(x) = A \sin\left(\frac{2\pi x}{2L/n}\right) = A \sin\left(\frac{n\pi x}{L}\right)$

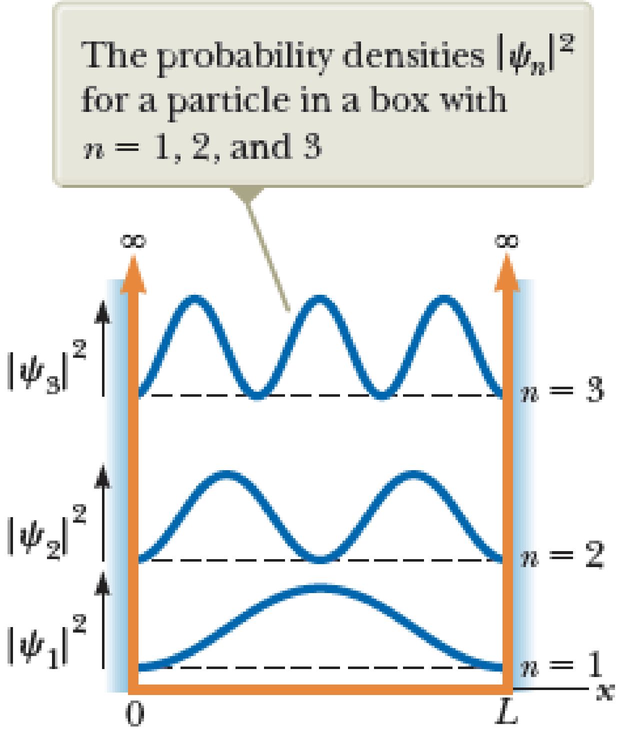
$A = \sqrt{2/L}$

$$\psi_n(x) = A\sin\left(\frac{2\pi x}{2L/n}\right) = A\sin\left(\frac{n\pi x}{L}\right)$$

Normalization of this function gives:

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$





a negative value for probability density would be meaningless, so it is positive always

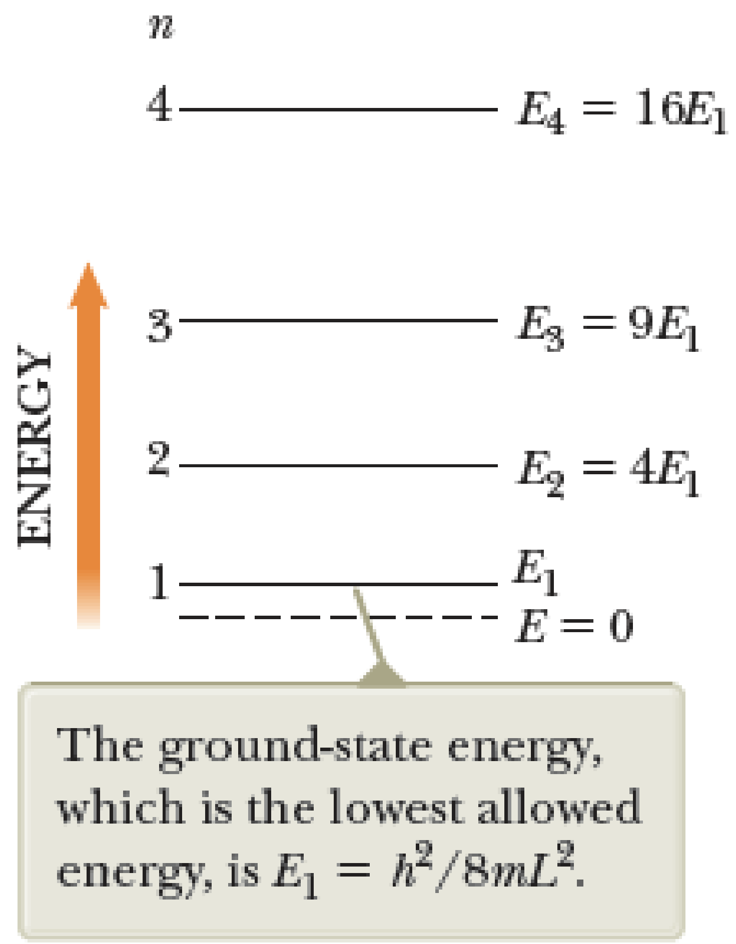
Because the wavelengths of the particle are restricted by the condition $\lambda = \frac{2L}{n}$

the magnitude of the momentum of the particle is also restricted to specific values →

$$p = \frac{h}{\lambda} = \frac{h}{2L/n} = \frac{nh}{2L}$$

$$E_n = \tfrac{1}{2}mu^2 = \frac{p^2}{2m} = \frac{(nh/2L)^2}{2m}$$

$$E_n = \left(\frac{h^2}{8mL^2}\right)n^2 \qquad n = 1, 2, 3, \ldots$$

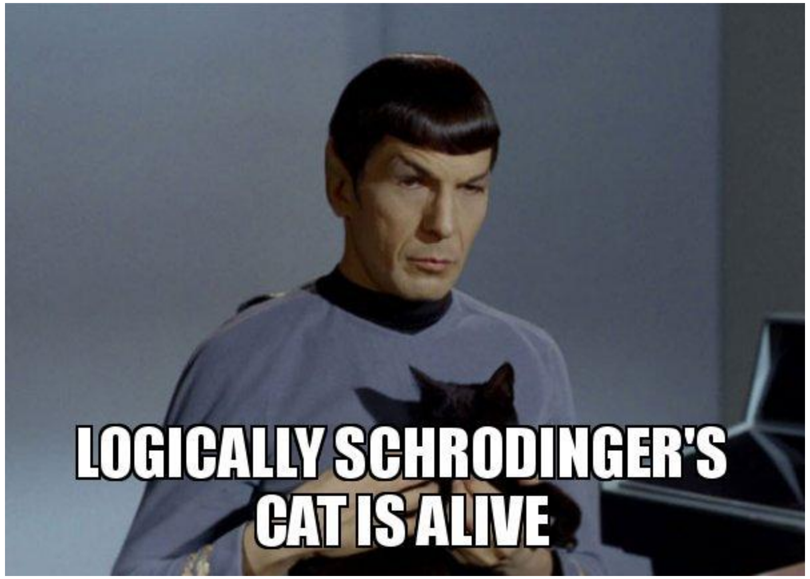


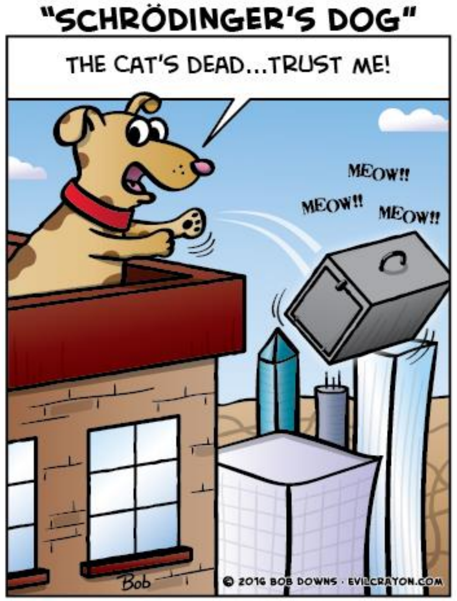
This expression shows that the energy of the particle is **quantized**.

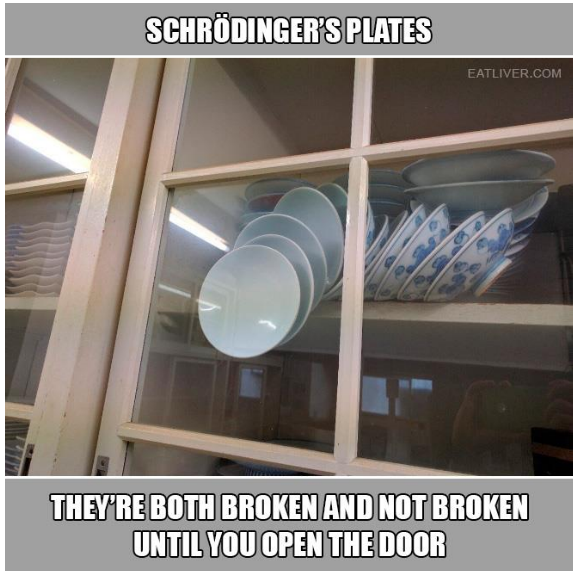
The lowest allowed energy corresponds to the **ground state**, which is the lowest energy state for any system.

Excites states → $E_n = n^2 E_1$

The Schrödinger Equation







The wave equation for material particles is different from that associated with photons because material particles have a nonzero rest energy.

The appropriate wave equation for a material particle was developed by Schrödinger in 1926.

The Schrödinger equation as it applies to a particle of mass *m* confined to moving along the *x* axis and interacting with its environment through a potential energy function *U(x)*;

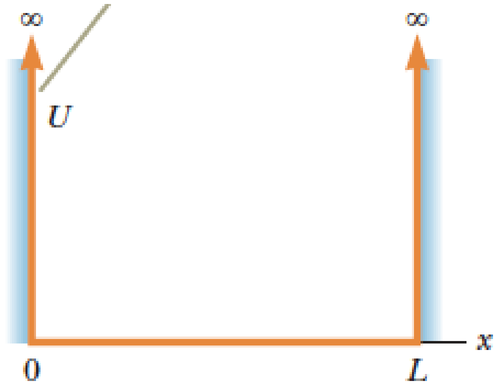
time-independent Schrödinger equation –>

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

E is a constant equal to the total energy of the system (the particle and its environment)

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

Let's go back to the particle an a box…



Because of the shape of this box, the particle in a box is sometimes said to be in a **square well** ☺

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

In the region $0 < x < L$, where $U = 0$, we can express the Schrödinger equation in the form

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi \qquad \text{where} \qquad k = \frac{\sqrt{2mE}}{\hbar}$$

The solution to this equation is a function **ψ** whose second derivative is the negative of the same function multiplied by a constant k^2. Both the sine and cosine functions satisfy this requirement. Therefore, the most general solution to the equation is a linear combination of both solutions:

$$\psi(x) = A \sin kx + B \cos kx$$

$$\psi(x) = A\sin kx + B\cos kx$$

The first boundary condition on the wave function is that $\psi(0) = 0$:

$$\psi(0) = A\sin 0 + B\cos 0 = 0 + B = 0$$

which means that $B = 0$. Therefore, our solution reduces to

$$\psi(x) = A\sin kx$$

The second boundary condition, $\psi(L) = 0$, when applied to the reduced solution gives

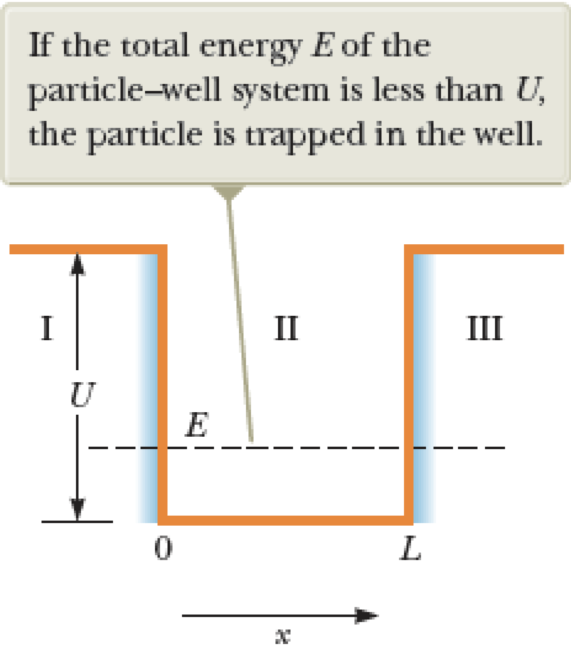
$$\psi(L) = A\sin kL = 0$$

$$kL = \frac{\sqrt{2mE}}{\hbar}L = n\pi$$

$$E_n = \left(\frac{h^2}{8mL^2}\right)n^2 \qquad \psi_n(x) = A\sin\left(\frac{n\pi x}{L}\right)$$

We obtain same result as we discussed before …

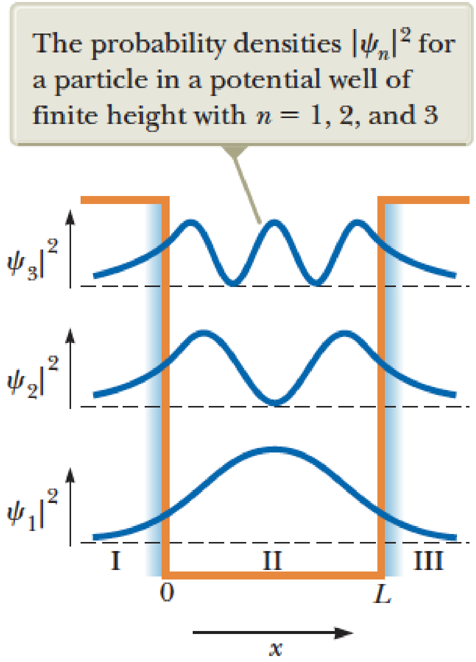
A Particle in a Well of Finite Height



consider a particle in a finite potential well, that is, a system having a potential energy that is zero when the particle is in the region 0 < x < L and a finite value U when the particle is outside this region

Classically → If the particle were outside the well, its kinetic energy would have to be negative, which is an impossibility

According to QM → a finite probability exists that the particle can be found outside the well even if E < U. (due to the the uncertainty principle)



The Schrödinger equation for regions I and III may be written

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

Because $U > E$, the coefficient of ψ on the right-hand side is necessarily positive.

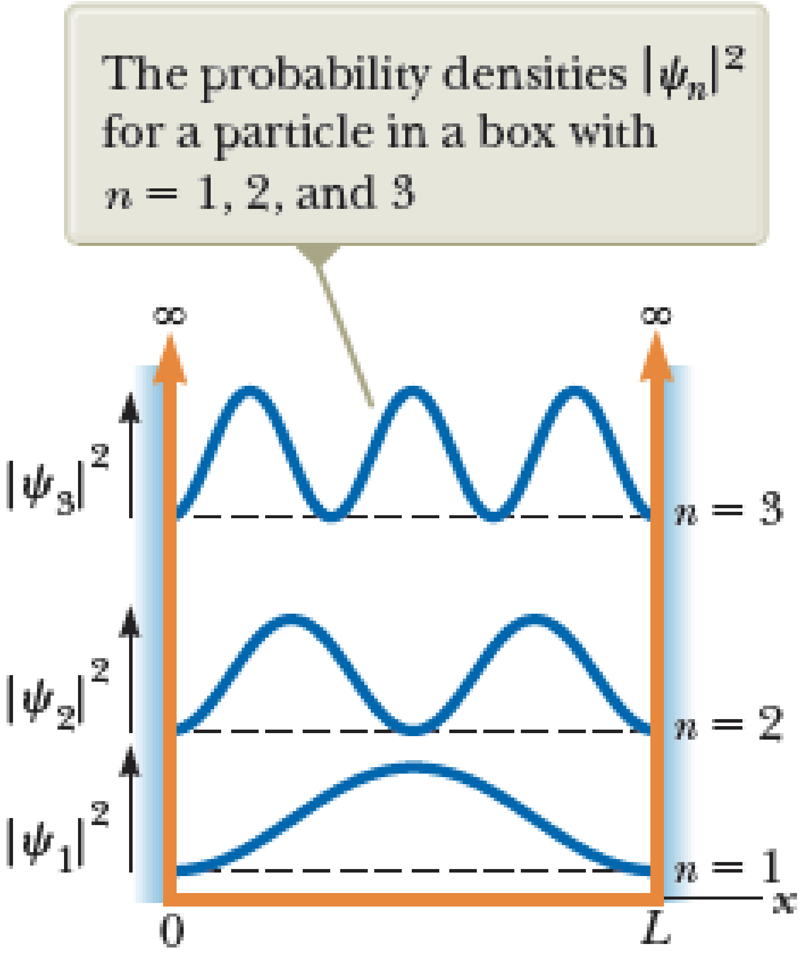
$$\frac{d^2\psi}{dx^2} = C^2\psi$$

General solutions:

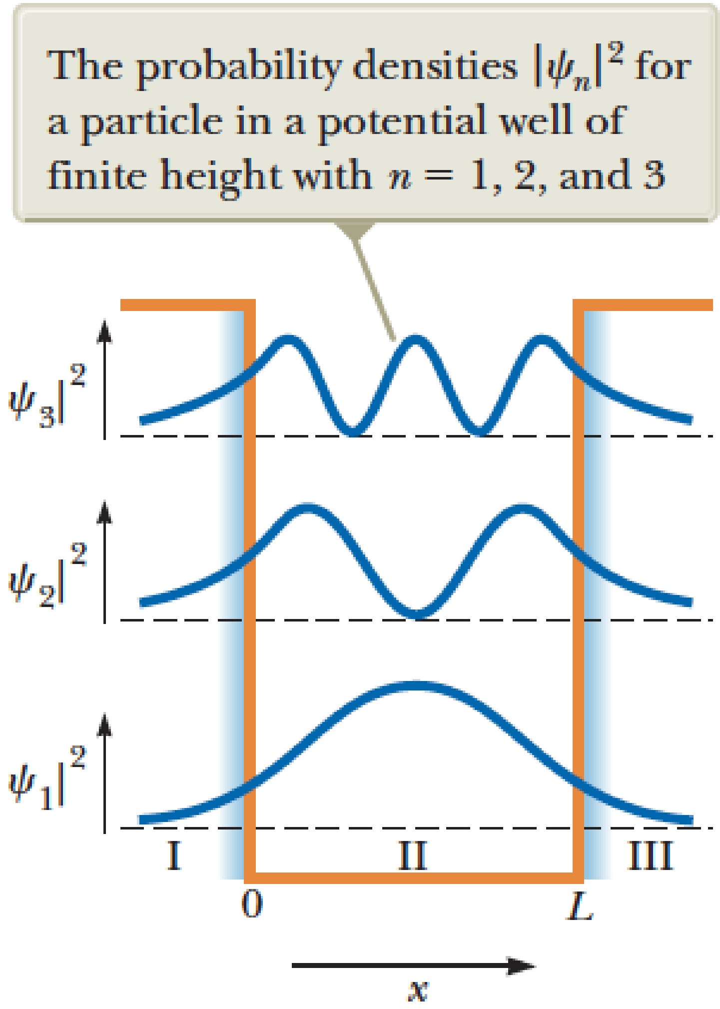
$$\psi_{\text{I}} = Ae^{Cx} \qquad \text{for } x < 0$$

$$\psi_{\text{III}} = Be^{-Cx} \qquad \text{for } x > L$$

$$\psi_{\text{II}}(x) = F\sin kx + G\cos kx$$

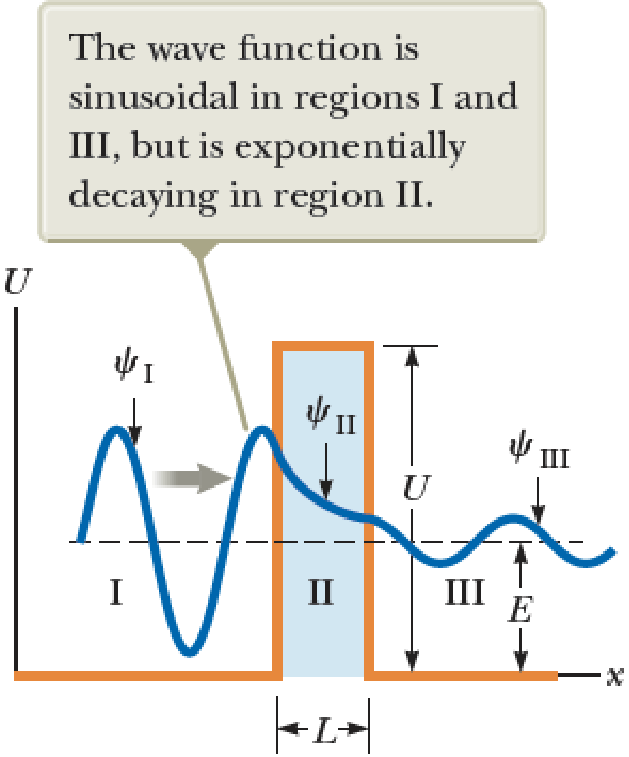


Particle in a box
(infinite height)



Particle in a potential well of a
finite height

Tunneling Through a Potential Energy Barrier



Suppose a particle of energy E < U is incident on the barrier from the left

Classically → the particle is reflected by the barrier.

If the particle were located in region II, its kinetic energy would be negative, which is not classically allowed.

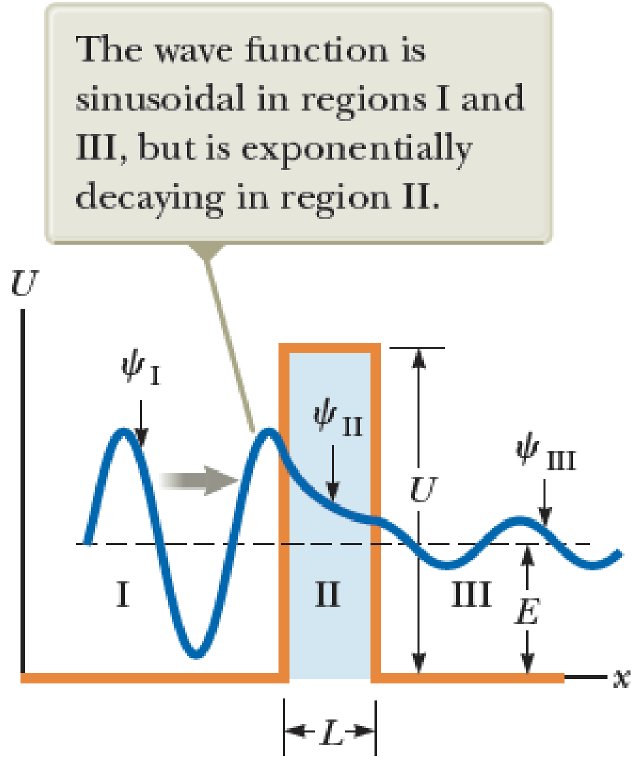
So, region II and therefore region III are both classically forbidden to the particle incident from the left.

According to QM → all regions are accessible to the particle, regardless of its energy!!!

Although all regions are accessible, the probability of the particle being in a classically forbidden region is very low.

transmission coefficient (T) : the probability that the particle penetrates to the other side of the barrier

reflection coefficient (R): the probability that the particle is reflected by the barrier



Because the incident particle is either reflected or transmitted; $T + R = 1$

$$T \approx e^{-2CL}$$

$$C = \frac{\sqrt{2m(U - E)}}{\hbar}$$

Applications of Tunneling:

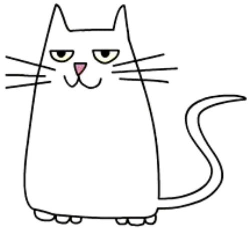
Tunnel diodes
Josephson junctions
Alpha decays
Sun energy
Quantum well
STM (scanning tunneling microscope)

Repeat the issue and try to solve these questions:

1) Consider an electron in an infinite potential well of width $10A^{o}$. Find the energies of first three energy levels in eV units.

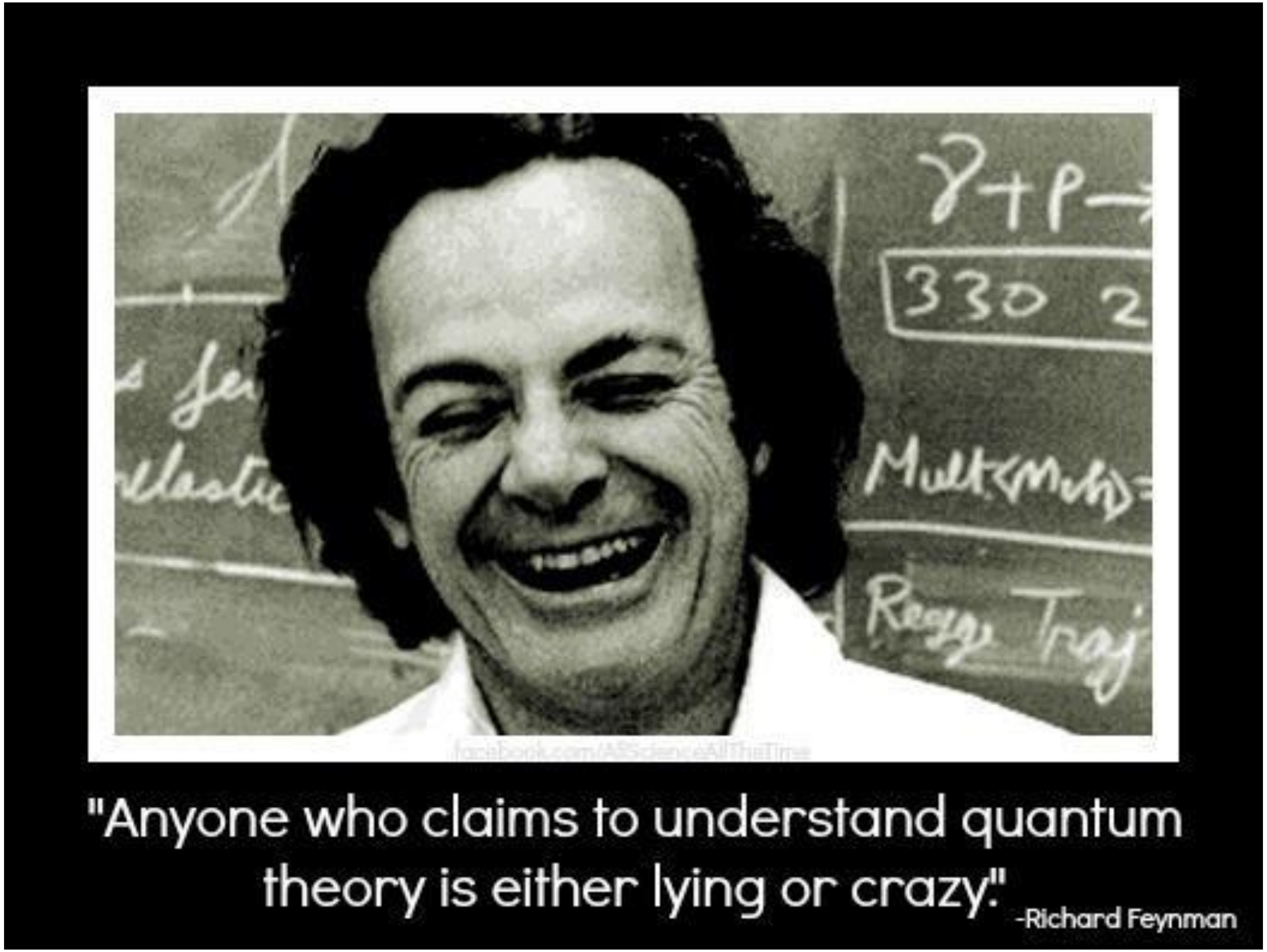
$$E_n = \left(\frac{h^2}{8mL^2}\right)n^2 \quad n = 1, 2, 3, \ldots$$

2) Width of the infinite potential well is 100 A^{o}. The lowest energy level of a particle in this well is 0.025 eV. Find the mass of the particle?



Homework:

Scrödinger’s Cat


"Anyone who claims to understand quantum theory is either lying or crazy."
-Richard Feynman