Chapter 4

QUANTUM MECHANICS

- **OBJECTIVES:**
  - To learn the application of Schrödinger equation to a bound particle and to learn the quantized nature of the bound particle, its expectation values and physical significance.
  - To understand the tunneling behavior of a particle incident on a potential barrier.
  - To understand the behavior of quantum oscillator.

An Interpretation of Quantum Mechanics

For an electromagnetic radiation, the probability of finding a photon per unit volume is related to the amplitude E of the electric field as

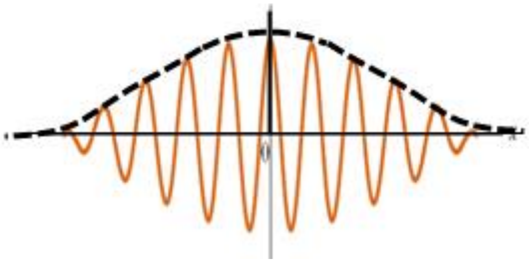
$$\frac{\text{PROBABILITY}}{V} \propto E^2$$

Similarly

ψ = wave function of a particle

= amplitude of the de Broglie wave

= probability amplitude



Time dependent wave function for a system:

$$\Psi(r_j,t) = \psi(r_j)\, e^{-i\omega t}$$

r_j is the position vector of the j^{TH} particle in the system.

ψ contains all the information about the particle

ψ $\rightarrow$ imaginary entity

$\rightarrow$ no physical significance

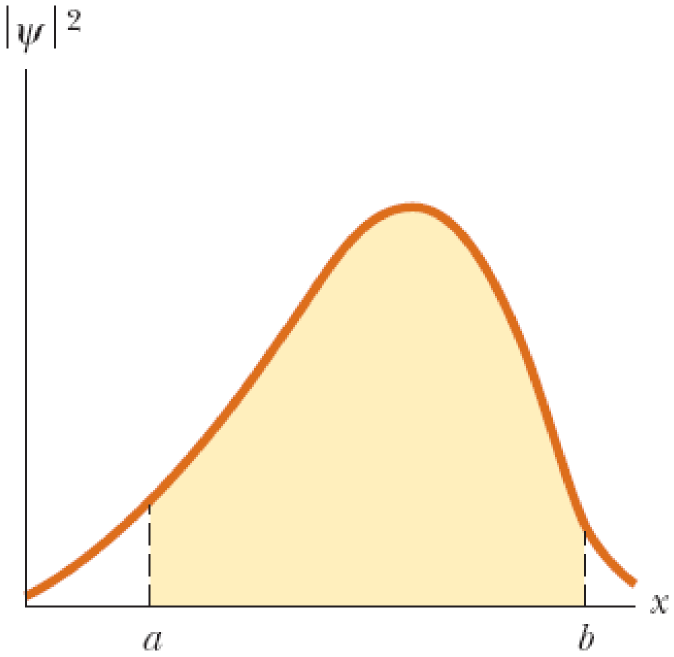
PROBABILITY DENSITY = $|\psi|^2$

$|\psi|^2$ $\rightarrow$ real and positive

$\rightarrow$ relative probability per unit volume that the particle will be found at any given point in the volume

$$P_{ab} = \int_a^b |\psi|^2 \, dx$$

= area under the probability density curve from a to b.



Normalization condition:

$$\int_{-\infty}^{\infty} |\psi|^2 \, dx = 1$$

Mathematical features of a physically reasonable wave function $\psi(x)$ for a system:

(i) $\psi(x)$ may be a complex function or a real function, depending on the system;

(ii) $\psi(x)$, must be finite, continuous and single valued everywhere;

(iii) The space derivatives of ψ, must be finite, continuous and single valued everywhere;

(iv) ψ must be normalizable.

- Measurable quantities of the particle (energy, momentum, etc) can be derived from ψ
- $\langle x \rangle$ = expectation value of x (i.e. the average position at which one expects to find the particle after many measurements)

$$\langle x \rangle \equiv \int_{-\infty}^{\infty} \psi^* x \, \psi \; dx$$

- The expectation value of any function $f(x)$ associated with the particle is

$$\langle f(x) \rangle \equiv \int_{-\infty}^{\infty} \psi^* f(x) \, \psi \; dx$$

Time independent Schrödinger equation

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

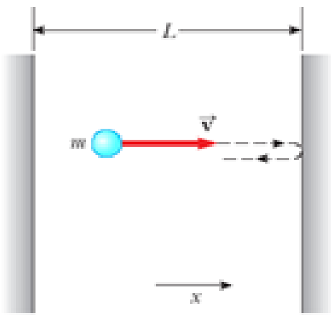
for a particle of mass m confined to moving along x axis and interacting with its environment through a potential energy function $U(x)$ and E = total energy of the system (particle and its environment)

Particle in an Infinite Potential Well (Particle in a "Box")

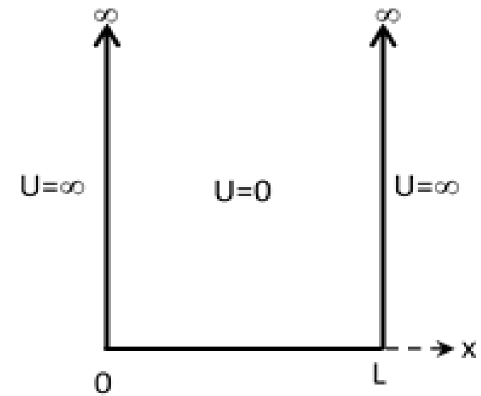
U(x) = o, for o < x < L,

U (x) = ∞ , for x < o, x > L

U (x) = ∞ , for x < o, x > L [here ψ(x) = o]



(a)



(b)

In o < x < L, U = o, the Schrödinger equation is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\psi = 0$$

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

ψ(x) = A sin(kx) + B cos(kx) where A and B are constants

At x = o, ψ = o So, o = A sin o + B cos o or **B = o** ,

At x = L , ψ = o ,

o = A sin(kL) + B cos(kL) = A sin(kL) + o , since $A \neq 0$, $\sin(kL) = 0$.

$\therefore \quad kL = n\pi; \quad (n = 1, 2, 3, \ldots\ldots\ldots)$

$$k = \frac{2\pi}{\lambda} = \frac{n\pi}{L} \quad \text{or} \quad L = n\left(\frac{\lambda}{2}\right)$$

$$k = \frac{\sqrt{2mE}}{\hbar}, \quad \therefore \quad kL = \frac{\sqrt{2mE}}{\hbar}L = n\pi$$

Each value of the integer n corresponds to a quantized energy value, E_n, where

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

The lowest allowed energy $(n = 1)$, $\quad E_1 = \dfrac{h^2}{8mL^2}$

E_1 is the ground state energy for the particle in a box

Excited states $\rightarrow \quad n = 2, 3, 4, \cdots$

Energies: $E_n \rightarrow 4E_1, 9E_1, 16E_1, \cdots$.

To find the constant A, apply normalization condition

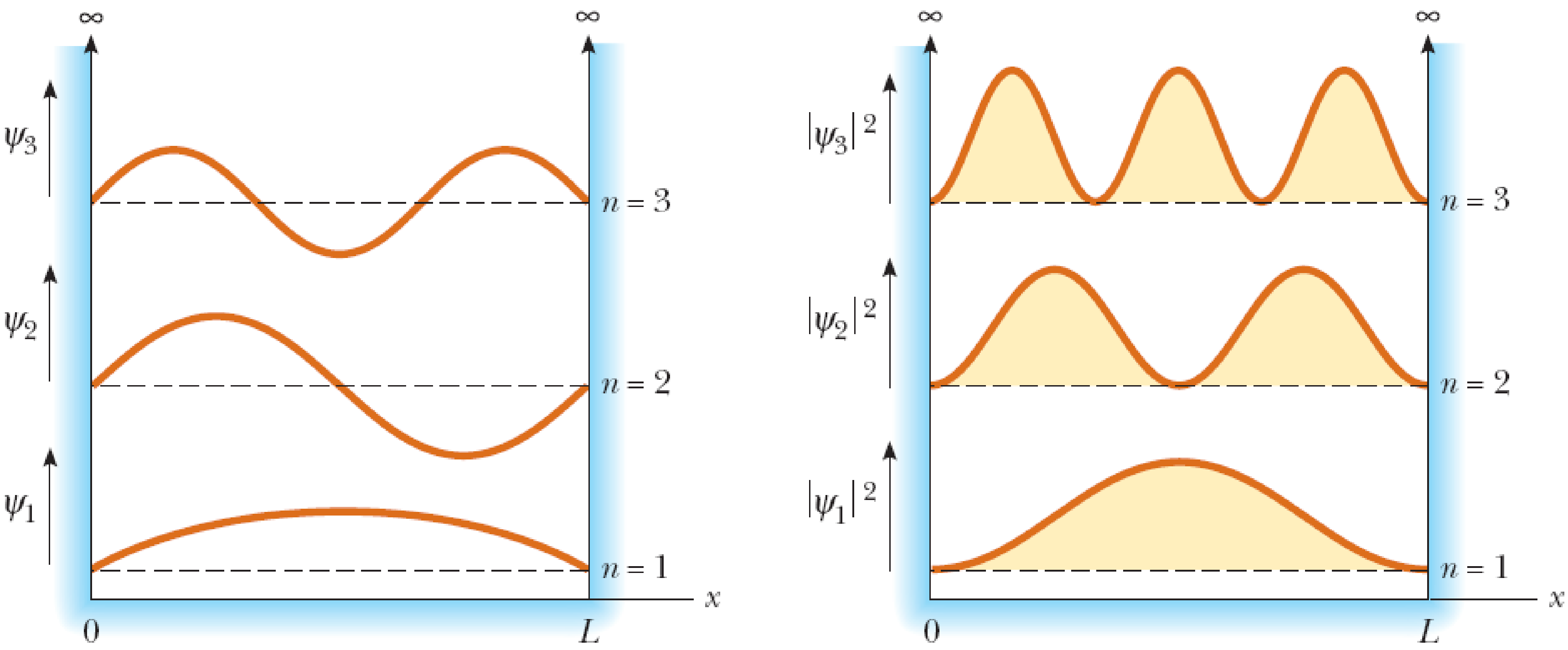
$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1 \quad \text{or} \quad \int_0^L A^2 \left[\sin\left(\frac{n\pi x}{L}\right)\right]^2 dx = 1$$

$$A^2 \int_0^L \frac{1}{2}\left[1 - \cos\left(\frac{2n\pi x}{L}\right)\right] dx = 1$$

Solving we get $A = \sqrt{\frac{2}{L}}$

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

PROBABILITY DENSITY $P_n(x) = \frac{2}{L} \sin^2\left(\frac{n\pi x}{L}\right)$



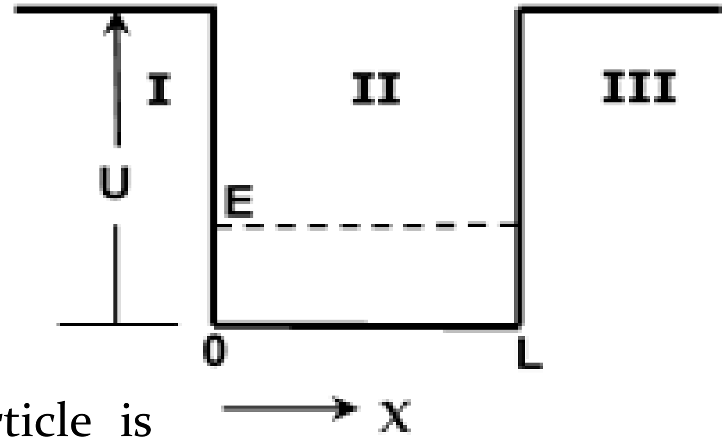
Sketch of (a) wave function, (b) Probability density for a particle in potential well of infinite height

A Particle in a Potential Well of Finite Height

A particle is trapped in the well. The total energy E of the particle-well system is less than U

$U(x) = 0, \quad 0 < x < L,$

$U(x) = U, \quad x < 0, \quad x > L$



- Particle energy E < U ; classically the particle is permanently bound in the potential well.
- However, according to quantum mechanics, a finite probability exists that the particle can be found outside the well even if E < U.
- The Schrödinger equation outside the finite well in regions I and III is:

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(U - E)\psi = C^2\psi \qquad \text{where} \quad C^2 = \frac{2m}{\hbar^2}(U - E)$$

General solution of the above equation is

$$\psi(x) = A\, e^{Cx} + B\, e^{-Cx}$$

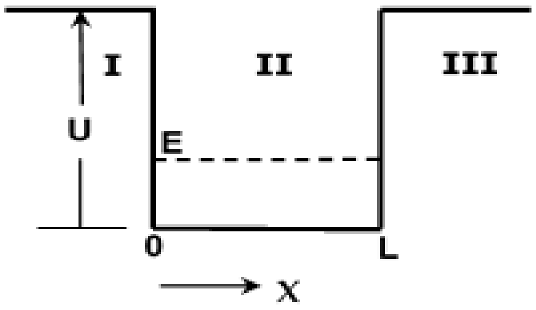
In region I, B = o;

$$\psi_I = A\, e^{C x} \qquad \text{for } x < 0$$

In region III, A = o;

$$\psi_{III} = B\, e^{-C x} \qquad \text{for } x > L$$

In region II,



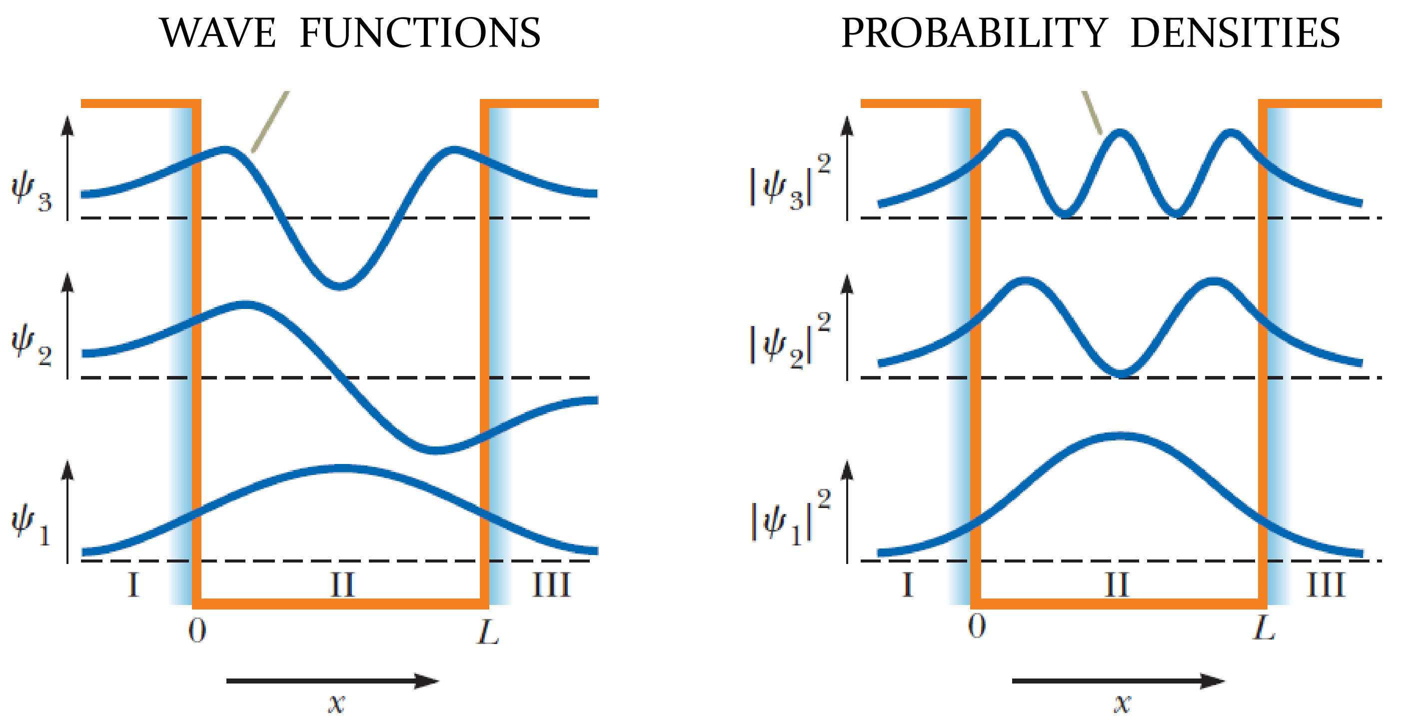
$$\frac{d^2\psi_{II}}{dx^2} + \underbrace{\left(\frac{2m}{\hbar^2} E\right)}_{k^2}\psi_{II} = 0$$

$$\psi_{II} = F \sin kx + G \cos kx$$

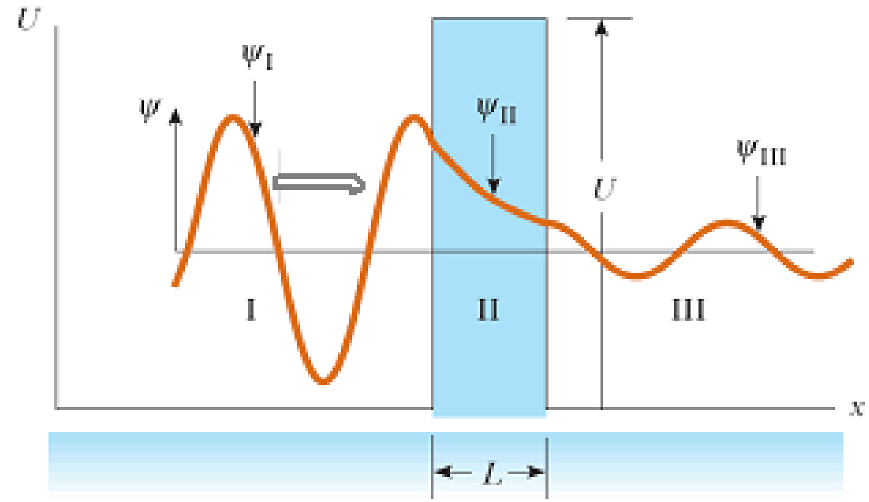
A, B, F, G values can be obtained by applying boundary conditions.

$$\psi_{I}(0) = \psi_{II}(0) \qquad \psi_{II}(L) = \psi_{III}(L)$$

$$\left.\frac{d\psi_{I}}{dx}\right|_{x=0} = \left.\frac{d\psi_{II}}{dx}\right|_{x=0} \qquad \left.\frac{d\psi_{II}}{dx}\right|_{x=L} = \left.\frac{d\psi_{III}}{dx}\right|_{x=L}$$



Tunneling Through a Potential Energy Barrier



- Consider a particle of energy E approaching a potential barrier of height U, ($E<U$).
- Since $E<U$, classically the regions II and III shown in the figure are forbidden to the particle incident from left.
- But according to quantum mechanics, all regions are accessible to the particle, regardless of its energy.
- An approximate expression for the transmission coefficient, when $T<<1$ is

$$T \approx e^{-2CL}, \quad \text{where } C = \frac{\sqrt{2m(U-E)}}{\hbar}$$

- Since the particles must be either reflected or transmitted:

$$R + T = 1$$

The Simple Harmonic Oscillator

- Consider a particle that is subject to a linear restoring force $F = -kx$, where k is a constant and x is the position of the particle relative to equilibrium (at equilibrium position x=0).
- Classically, the potential energy of the system is,

$$U = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2$$

where the angular frequency of vibration is $\omega = \sqrt{k/m}$.

- The total energy E of the system is,

$$E = \ Kinetic\ Energy + Potential\ Energy = K + U = \frac{1}{2}kA^2 = \frac{1}{2}m\omega^2 A^2$$

where A is the amplitude of motion.

- A quantum mechanical model for simple harmonic oscillator can be obtained by substituting $U = \frac{1}{2}m\omega^2 x^2$ in Schrödinger equation:

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

- The solution for the above equation is

$$\psi = Be^{-Cx^2}$$

where $C = m\omega/2\hbar$ and $E = \frac{1}{2}\hbar\omega$.

- Energy of a state is given by

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega; \qquad n = 0, 1, 2 \dots.$$

- The state n=o corresponds to the ground state, whose energy is $E_0 = \frac{1}{2}\hbar\omega$