

# UNIT 4 QUANTUM MECHANICS

1

## LECTURE 7

# What we learned so far about Quantum mechanics?

## 1. We had a short walk down the memory lane (1900-1927)

- ✓ Classical mechanics, relativistic mechanics, quantum mechanics and quantum field theory
- ✓ Hertz, Planck, Einstein, Bohr, Crompton, Raman, de Broglie, Heisenberg, Schrödinger, Dirac, Pauli, Born
- ✓ Development of quantum mechanics

## 2. Classical mechanics Explained

Newton's corpuscular concepts of light-particles

Maxwell's wave concepts of light from EM theory

Reflection, refraction –explained through particle concept-ray optic

Interference, diffraction, polarization– wave nature

It was all about light!

### 3. How QM concept helped in overcoming classical limitation?

**Black body radiation** ,

Wien and Rayleigh-Jean formula,

UV catastrophe

Planck's quantum oscillator,

$$I_{\nu} d\nu = \frac{8\pi \nu^2}{c^3} kT d\nu$$

$$I_{\nu} d\nu = \frac{A \nu^3}{c^4} e^{-B\nu/T} d\nu$$

$$I_{\nu} d\nu = \frac{8\pi h}{c^3} \frac{\nu^3 d\nu}{e^{h\nu/kT} - 1}$$

**Photoelectric effect**,

Hertz's discovery

Einstein's photoelectric equation,

The name photon

$$E_k = h\nu - h\nu_0$$

$\phi_m$ -Work function

**Compton effect**-scattering of light by electron

**Raman effect**-vibration spectra of molecules upon photon irradiation

**All these phenomenon were successfully explained by QM**

4. Characteristic properties of a wave : **v and  $\lambda$**

5. Characteristic properties of a particle: **p and E**

6. Radiation (wave)-particle dual nature

$$p = mc = \frac{h}{\lambda}$$

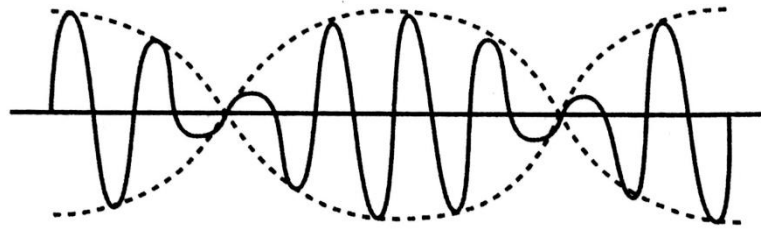
7. Matter (particle) –wave dual nature

$$\lambda = \frac{h}{mv} = \frac{h}{p}$$

De Broglie's hypothesis;  
connecting the wave nature  
with particle nature through  
the Planck's constant..

Used Einstein's famous  
mass-energy relation  
 $E=mc^2$

8. Various relation connecting the de Broglie wavelength  
associated with a particle of mass m and having energy E



## 9. Characteristics of matter wave

## 10. Wave velocity, phase velocity, group velocity and particle velocity

$$v_p = \frac{\omega}{k} \quad v_g = \frac{\Delta\omega}{\Delta k} \quad \therefore v_g = -\frac{\lambda^2}{2\pi} \frac{\partial\omega}{\partial\lambda}$$

$v$  particle velocity

$$\frac{df}{dx} = \lim_{\Delta x \rightarrow 0} \frac{\Delta y}{\Delta x}$$

non-dispersive-  
normal-dispersive-  
anomalous dispersive mediums-

$$v_p = v_g$$

$$v_p > v_g$$

$$v_p < v_g$$

## 11. Relationship between $v_g$ and $v_p$ & $v_g$ and $v$

$$v_g = v_p - \lambda \frac{dv_p}{d\lambda}$$

→ Dispersion

$$v_g = v$$

## 12. Heisenberg uncertainty principle

Wave-particle duality introduce the concept of uncertainty. This concept suggest that if the particle nature of the matter becomes certain, the wave nature becomes uncertain and vice versa.

### Uncertainty in the measurements of physical quantities

There are three **conjugate variables** of great importance in **quantum mechanics**: position and momentum, angular orientation and angular momentum, and energy and time.

1.  $\Delta p \Delta x \geq \hbar$       Original statement of Heisenberg uncertainty principle
2.  $\Delta E \Delta t \geq \hbar$       Time –Energy uncertainty principle
3.  $\Delta L_{\theta} \Delta \theta \geq \hbar$       Angular momentum -Angular orientation uncertainty principle

### 13. Applications of Heisenberg uncertainty principle are

1. Non existence of electron in the nucleus
2. Existence of proton, neutrons and  $\alpha$ -particles in the nucleus
3. Binding energy of an electron in an atom
4. Radius of Bohr's first orbit
5. Energy of a particle in a box
6. Ground state energy of the linear harmonic oscillator
7. Radiation of light from an excited atom

## 14. Wave Equation and function- Classical

$$\nabla^2 u = \frac{1}{v^2} \frac{\partial^2 u}{\partial t^2} \quad u = a \sin(\omega t - kx)$$

Where 'u' is the wave function... that is the solution of the wave equation

e.g, u can be E, B or P at a position (x,y,z) at a given time t.

## 15. Wave function- Quantum

The characteristics of the wave functions in quantum mechanics are

➤  $\psi$  must be finite, continuous and single valued everywhere

➤  $\psi$  must be normalizable  $\iiint_{-\infty}^{\infty} \psi^* \psi \, dV = 1$

➤ also  $\frac{\partial \psi}{\partial x}, \frac{\partial \psi}{\partial y}, \frac{\partial \psi}{\partial z}$  must be finite, continuous and single valued



## 18. Schrödinger wave equation

Schrödinger time- independent wave equation for free particle

$$\nabla^2 \psi + \frac{2mE}{\hbar^2} \psi = 0$$

Schrödinger time- independent wave equation

$$\nabla^2 \psi + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

Schrödinger time- dependent wave equation

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V \right] \psi = i\hbar \frac{\partial \psi}{\partial t}$$

$$\mathbf{H}\psi = \mathbf{E}\psi$$

## 19. Operators, Eigen value and Eigen function

Classical expression  
for total energy

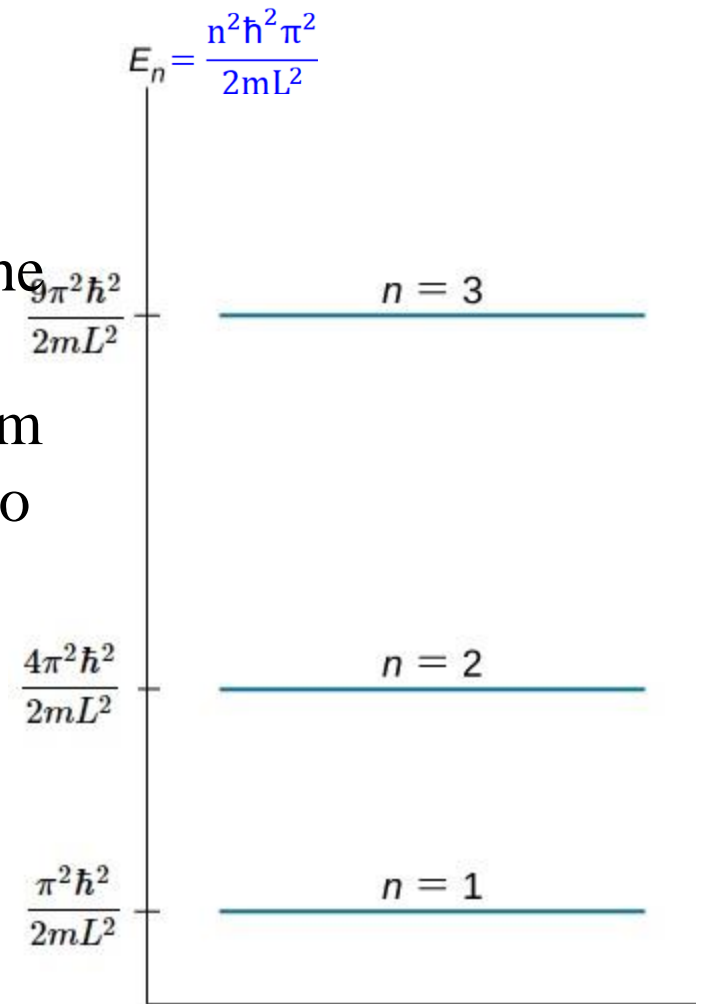
$$\frac{p^2}{2m} + V = E$$

$$E = i\hbar \frac{\partial}{\partial t}$$
$$p = -i\hbar \nabla$$

## 20. Particle in a box- Eigen value

- **E** is the Eigen value of the particle in the potential well
- Constitute the energy level of the system
- **n** is the quantum number corresponds to the energy level **E<sub>n</sub>**

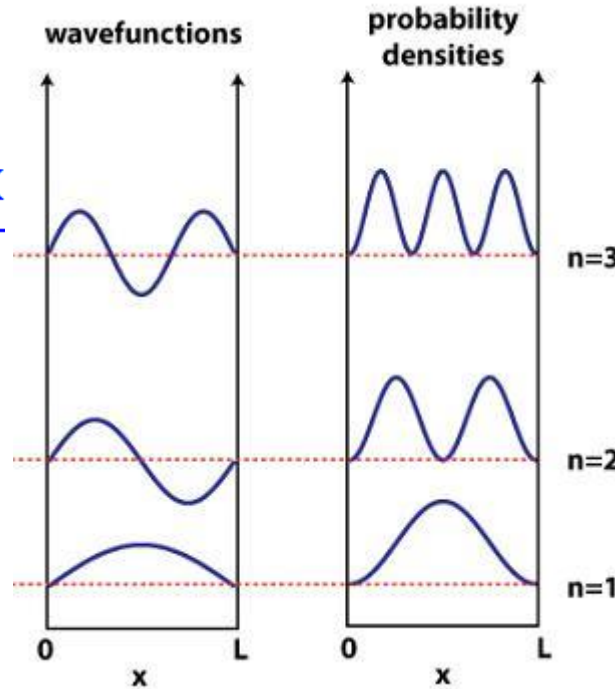
$$E_n = \frac{n^2 \hbar^2 \pi^2}{2mL^2}$$



So we found out the energy (**Eigen value**) of the particle in a box, with the help of Schrödinger equation

## 21. Particle in a box- Eigen Function

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



Probability of finding the particle is

$$|\psi_n(x)|^2$$

- Classical mechanics predict the same probability to find the particle anywhere in the box
- But quantum mechanics different probability
- There are points where particle will never present
- Probability is different also with energy of the particles

The characteristics of the wave functions in quantum mechanics are

- a)  $\psi$  must be finite, continuous and single valued everywhere
- b)  $\psi$  must be normalizable
- c)  $\psi$  must be finite, continuous and single valued
- d) All of the above

**Ans: D**

When a Laplacian operator ( $\nabla^2$ ) and Energy (E) operate on wave function ( $\Psi$ ), we get the wave equation  $\nabla^2 \psi + \frac{2m}{\hbar^2} (E - V) \psi = 0$ , What type of equation is it?

- a) Time dependent Schrodinger equation
- b) Time-independent Schrodinger equation for any particle
- c) Time-independent Schrodinger equation for free particle
- d) None of the above

**Ans: B**

The energy of a particle at a level  $n$  in infinite potential well is

- (a) Proportional to  $n^2$
- (b) Proportional to  $n$
- (c) Inversely proportional to  $n^2$
- (d) Inversely proportional to  $n$

**Ans: A**

The momentum of a particle in infinite potential well is

- (a) Proportional to  $n^2$
- (b) Proportional to  $n$
- (c) Inversely proportional to  $n^2$
- (d) Inversely proportional to  $n$

**Ans: B**

The momentum of a particle in infinite potential well of length  $L$  is

- (a) Proportional to  $L^2$
- (b) Proportional to  $L$
- (c) Inversely proportional to  $L^2$
- (d) Inversely proportional to  $L$

**Ans: D**



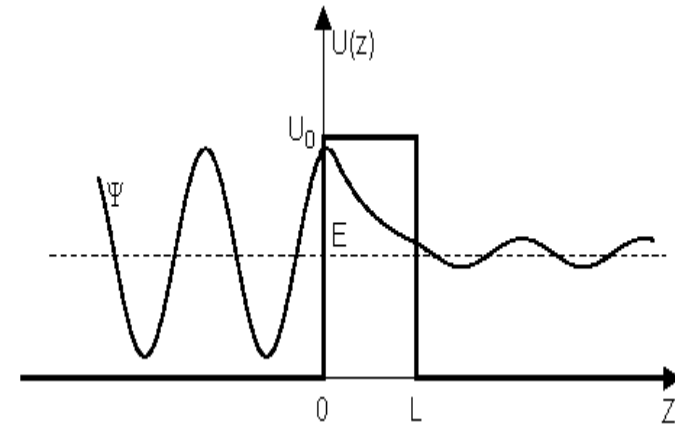
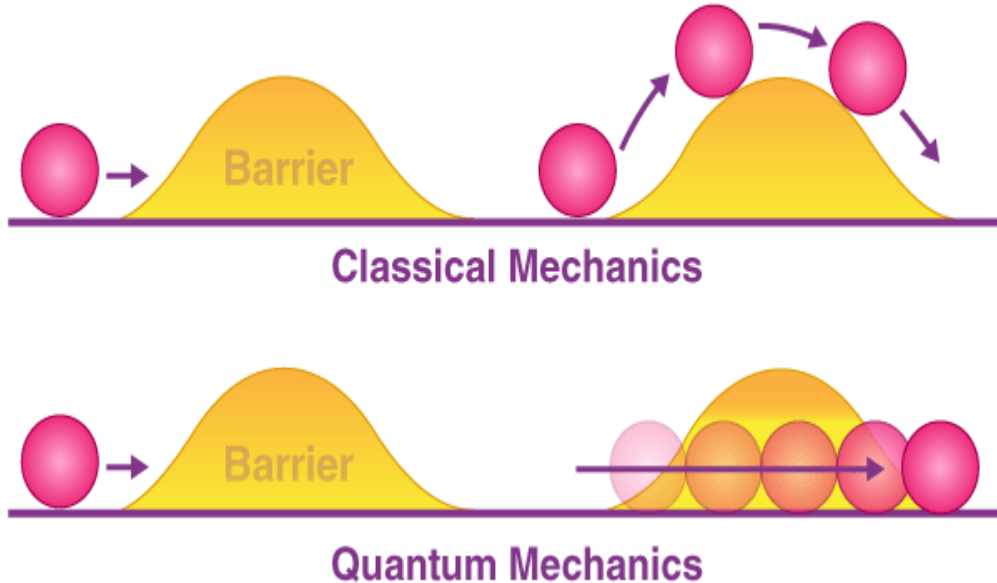
The Energy of a particle in infinite potential well of length  $L$  is

- (a) Proportional to  $L^2$
- (b) Proportional to  $L$
- (c) Inversely proportional to  $L^2$
- (d) Inversely proportional to  $L$

Ans: C

# Tunneling

18



Found Application in

- ❖ **Quantum computing.**
- ❖ In Electronics-Limits the miniaturization of transistors.
- ❖ Nuclear fusion.
- ❖ Tunnel diodes (Esaki Diodes).
- ❖ Scanning tunneling microscopes.

# Quantum Tunneling- History

19

- Consequence of the wave nature of matter
- First used to explain alpha decay of heavier elements in 1928 by George Gamow
- Shown experimentally by Leo Esaki in 1958 in the tunneling diode

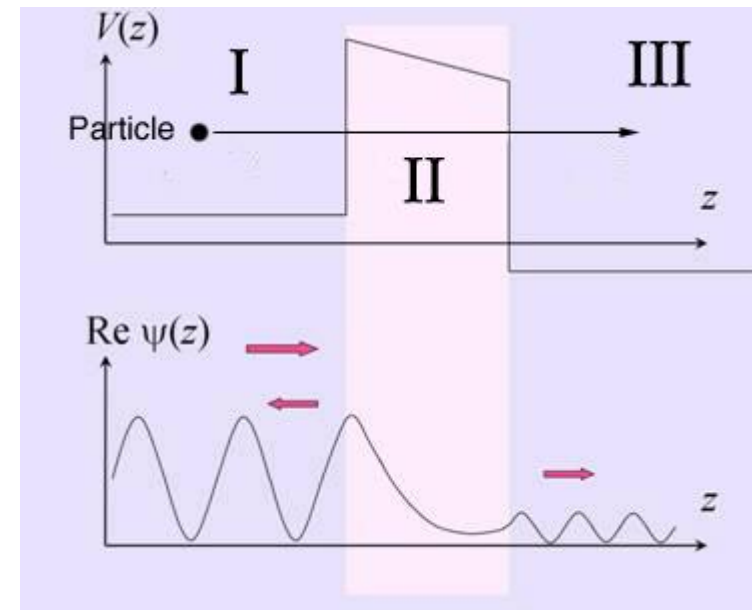
# What is Quantum Tunneling?

20

- ❑ At the quantum level, matter has corpuscular and wave-like properties
- ❑ Tunneling can only be explained by the wave nature of matter as described by quantum mechanics
- ❑ Classically, when a particle is incident on a barrier of greater energy than the particle, reflection occurs
- ❑ When described as a wave, the particle has a probability of existing within the barrier region, and even on the other side of it

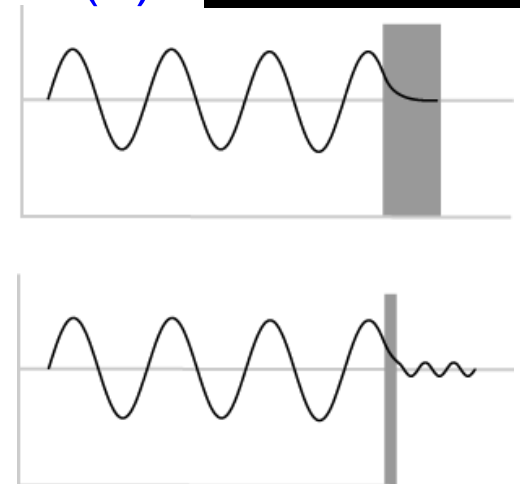
# How Can Tunnelling Be?

- ❖ Solutions to the wave equation have the general form (I)
- ❖ In the barrier region, the solution becomes (II)
- ❖ The wave function decays exponentially in the barrier region
- ❖ If some portion of the wave function still exists on the other side of the barrier, transmission has occurred
- ❖ The width of the barrier is the most prominent factor in determining the probability of transmission



$$(I) \quad Ae^{ikx} + Be^{-ikx}$$

$$(II) \quad Ce^{kx} + De^{-kx}$$



# UNIT 4-Quantum Mechanics

22

**Text Book: ENGINEERING PHYSICS by HITENDRA K MALIK AND A K SINGH, MCGRAW HILL EDUCATION, 1st Edition, (2009)**

## **References:**

- ENGINEERING PHYSICS by B K PANDEY AND S CHATURVEDI, CENGAGE LEARNING, 1st Edition, (2009).
- ENGINEERING PHYSICS by D K BHATTACHARYA, POONAM TONDON OXFORD UNIVERSITY PRESS.