Unit IV
Quantum Mechanics

Topics

1) Wavelength of matter waves in different forms

2) Heisenberg uncertainty principle

3) Concept of phase velocity and group velocity (qualitative)

4) Wave function and its significance

5) Tunneling Effect

Wavelength of matter waves in different forms

1) Let us consider E is the kinetic energy and v is velocity of a particle having mass "m" then

$$E = \frac{1}{2}mv^2 \qquad (1)$$

$Multiply\ and\ divide\ by\ mass\ "m"$

$$E = \frac{1}{2}\frac{m^2v^2}{m}$$

By using $p = mv = momentum$

$$E = \frac{1}{2}\frac{p^2}{m}$$

$$p = \sqrt{2mE}$$

1) De-Broglie wavelength for particle in Gaseous state.

According to kinetic theory of gases, the average KE of the particle is

$$E = \frac{3}{2}\ KT$$

$$K = 1.38 \times 10^{-23} J/k = Boltzmann's\ constant$$

$$T = Absolute\ temp.$$

We have $E = \frac{1}{2}\frac{p^2}{m}$

On comparing energy

$$\frac{1}{2}\frac{p^2}{m} = \frac{3}{2}\ KT$$

$$p = \sqrt{3mKT}$$

1) De-Broglie wavelength of an accelerated electron under “V”

The work done by electric field on the electron appears as the gain in its KE

$$E = eV$$

$Because$ $$E = \frac{1}{2}\frac{p^2}{m}$$

Therefore $$\frac{1}{2}\frac{p^2}{m} = eV$$

$$p = \sqrt{2meV}$$

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

$therefore$ $$\lambda = \frac{h}{\sqrt{2meV}}$$

$$\lambda = \frac{12.27}{\sqrt{V}}\text{Å}$$

Numerical on matter wave

Problem: Calculate the Wavelength of the Electron that is moving at the Speed of Light.

Sol:

λ= h / m v

M= mass of electron =9.1 * 10 (-31) Kg

$$\lambda = \frac{6.6260 \times 10^{-34} Js}{9.1 \times 10^{-31} Kg \times 3 \times 10^{8} ms^{-1}}$$

$$\Rightarrow \lambda = 0.2424 \text{ x } 10^{-11} \text{m}$$

Heisenberg uncertainty principle

- **Uncertainty principle**, also called **Heisenberg uncertainty principle** or **indeterminacy principle**, explained in 1927 by the German physicist Werner Heisenberg.
- Definition: Heisenberg's uncertainty principle states that it is impossible to measure or calculate exactly, both the position and the momentum of an object. This principle is based on the wave-particle duality of matter.
- Therefore, the position and the velocity of an object cannot both be measured exactly, at the same time, even in theory.

➢The complete rule stipulates that the product of the uncertainties in position and momentum is equal to or greater than a tiny physical quantity, or constant $h/(4\pi)$

$$\hbar = \frac{h}{2\pi}$$

Planck's constant

$$\Delta p \Delta x \geq \frac{h}{4\pi} \Rightarrow \Delta p\, \Delta x \geq \frac{1}{2}\hbar$$

uncertainty in position

uncertainty of momentum

Reduced Planck constant

➢A quite accurate measurement of one observable involves a relatively large uncertainty in the measurement of the other.

➢Momentum is a vector quantity and let p_x, p_y, p_z are momentum compnets along x, y, z directions

$$\Delta x \Delta p_x \geq \frac{h}{4\pi}, \qquad \Delta x \Delta p_y \geq \frac{h}{4\pi}, \qquad \Delta x \Delta p_y \geq \frac{h}{4\pi}$$

➢There is a other pair of quantities which can be found simultaneously

$$\Delta t \Delta E \geq \frac{h}{4\pi}$$ (Time and Energy)

$$\Delta L \Delta \theta \geq \frac{h}{4\pi}$$ (Angular Momentum and angle)

Problem: Calculate the uncertainty in the momentum of an electron if uncertainty in its position is 1 Å.

$\Delta x \Delta p \geq h/4\pi$

$\Delta p \geq h/4\pi\Delta x$

$\Delta p \geq 5.28 \times 10^{-25} \text{kg m s}^{-1}$

Concept of phase velocity/group velocity (qualitative)

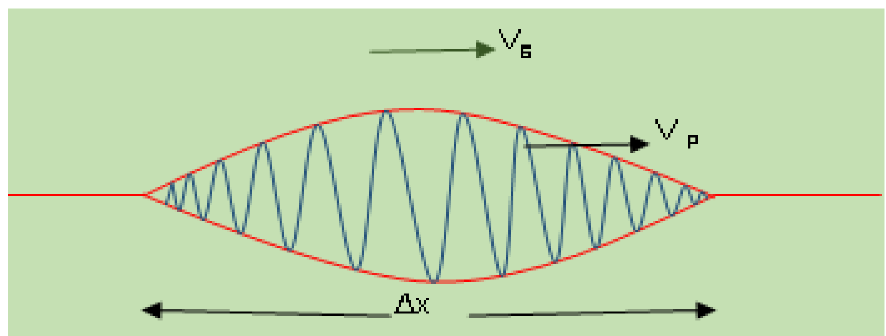
Wave: A wave is defined as a disturbance in a medium from an equilibrium condition that propagates from one region of medium to other regions.

Propagation of Wave: Wave propagate in the medium occurs with two different kinds of velocity. i.e. phase velocity and group velocity.

1. Phase Velocity (*Vp*): The velocity with which the phase of a wave propagates through the medium at a certain frequency is called the phase velocity or wave velocity.

Group Velocity (*Vg*): The velocity of propagation of **wave packet** through space is known as group velocity.

Wave Packet/Wave group: It is an **envelope** which contains a number of plane waves having a different wavelength. These numbers of waves superimpose on each other and a resultant wave obtain.



Let:

$$y = Asin\omega(t - \frac{x}{v})$$

Direction of disturbance

Amplitude of wave

Angular Frequency

Direction of propagation

Velocity of wave

$$y = A\sin\left(\omega t - \frac{\omega x}{v}\right)$$

The function $\omega(k)$, which gives ω as a function of k *(wave number)*, is known as the dispersion relation.

$$k = \frac{2\pi}{\lambda}$$

$$k = \omega / v$$

$$y = A\sin(\omega t - kx)$$

Here $(\omega t - kx)$= phase of wave

Differentiating phase w.r.t. 't'

$$\omega - k\, dx/dt = 0$$

$$dx/dt = \omega / k$$

$$dx/dt = V_p = \omega / k$$

For group velocity We can try by considering two waves

$$\frac{x}{t} = \frac{\delta\omega}{\delta k}$$

$$\boxed{V_g = \frac{\delta\omega}{\delta k}}$$

OR

$$\boxed{V_g = \frac{d\omega}{dk}}$$

Relation between phase velocity and group velocity

Group Velocity And Phase Velocity

The Group Velocity and Phase Velocity relation can be mathematically written as-

$$V_g = V_p + k\frac{dV_p}{dk}$$

Where,

- V_g is the group velocity.
- V_p is the phase velocity.
- k is the angular wavenumber.

Group Velocity and Phase Velocity relation for Dispersive wave non-dispersive wave

Type of wave	Condition	Formula
Dispersive wave	$\frac{dV_p}{dk} \neq 0$	$V_p \neq V_g$
Non-dispersive wave	$\frac{dV_p}{dk} = 0$	$V_p = V_g$

In a dispersive medium, waves of different frequencies travel at different speeds.

For example, the light wave which consist of seven colors when enters into a medium say prism then it splits into seven colors. Prism acts as a dispersive medium for light wave that is why the seven components of wave packet split depending upon their frequency.

*Note: If the wave speed depends **only** on the physical properties of the medium (the elastic and inertia properties of a mechanical medium, or the relative permeability and permittivity for EM waves) then the wave speed is a constant, independent of frequency. Such a medium is called a non-dispersive medium and waves traveling through this medium will maintain a constant shape.*

Wave-function of a matter wave

- **wave function**, in QM, is a variable quantity or equation that mathematically describes the wave characteristics of a particle.
- By analogy with waves such as those of sound, a wave function, designated by the Greek letter psi, Ψ, may be thought of as an expression for the amplitude of the particle wave (or de Broglie wave).
- Although such waves functions has no physical significance. But Ψ^2 have physical significance: the probability of finding the particle described by a specific wave function Ψ at a given point and time is proportional to the value of Ψ^2.

- Usually, it is used only to describe the behavior of ‘slow’ electrons **because it is not accurate for faster-moving** particles. Faster-moving particles, those moving at a few percentages of the speed of light or faster, are noticeably affected by Special Relativity.

- The wave function can include the imaginary number **i**, that is the square root of negative 1.

In this metaphor, the surfers represent electrons being guided by a wave.

Characteristics of Wave function

1) The wave function must be finite, continuous and single valued everywhere.

2) First order partial differentiation w.r.t. spatial coordinates of wave function must be finite, continuous and single valued everywhere.

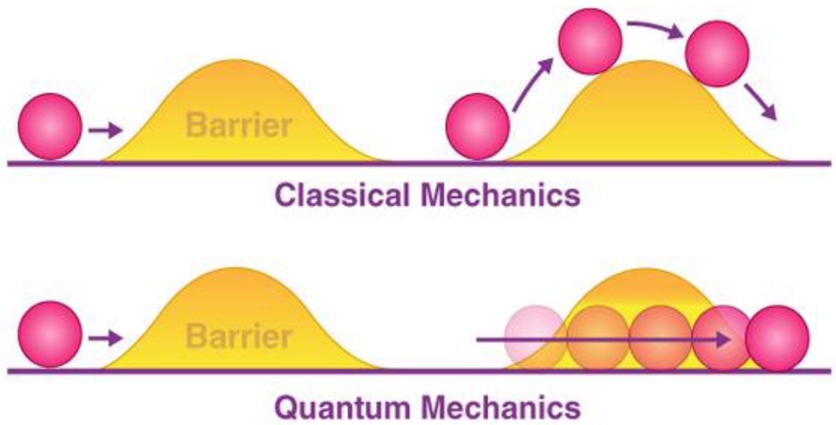
3) Wave function must be normalizable.

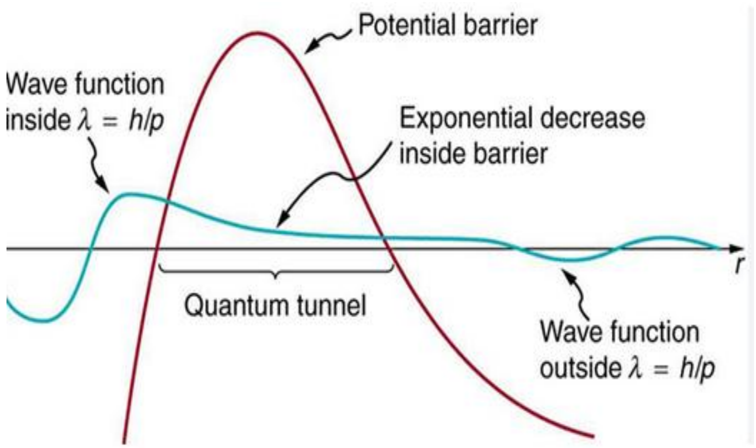
$$\int_{-\infty}^{\infty} \Psi^{*}\Psi dx=1$$

If Ψ is real function then $\int_{-\infty}^{\infty} |\Psi|^{2} dx=1$

Tunneling Effect

- In **quantum mechanics**:-To describe the system completely, an associated complex function is introduced in quantum mechanics (**the wave function**). The wave function, which is a function of time and all system particles position, is a solution of the wave Schrodinger equation. In order to use the system wave function, one should determine rather than wave function.
- Quantum tunneling is defined as a quantum mechanical process where wave functions can penetrate through a potential barrier. The transmission through the potential barrier can be finite and relies exponentially on the barrier width and barrier height. The wave functions have the genuine probability of disappearing on one side and reappearing on the remaining side.





- Quantum tunnelling is defined as a quantum mechanical process where wavefunctions can penetrate through a potential barrier.
- The wave functions have the genuine probability of disappearing on one side and reappearing on the remaining side. The first derivative of the wave functions is continuous.

Applications of Quantum Tunnelling

Nuclear Fusion, Scanning Tunnelling Microscope

THANK YOU……