Unit - 3

Quantum Mechanics – I		07
3.1	De-Broglie hypothesis and its various forms	
3.2	Heisenberg's uncertainty principle, its implications and application	
3.3	Wavefunction and its probabilistic interpretation, Condition of Normalization	

De-Broglie Broglie Hypothesis

Wave particle duality

- Interference, diffraction and polarization

$\Longrightarrow$ Explained by WAVE THEORY.

- Photoelectric effect, emission and absorption of light

$\Longrightarrow$ Explained by QUANTUM THEORY or PARTICLE THEORY.

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De-Broglie Broglie Hypothesis

(a). Matter and light, both are form of energy and each of them can be transformed into each other.

(b). Both are governed by the space time symmetries of the theory of relativity.

De Broglie Concept of Matter Wave: In 1924, Louis de Broglie proposed that the matter also possesses dual character like light. His concept about the dual nature of matter was based on the following facts,

Statement: "A moving matter particle is surrounded by a wave whose wavelength depends upon the mass of the particle and its velocity. The waves are known as *matter waves* or *de-Broglie waves*." Mathematically,

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

where h is Plank's constant and p is momentum of particle.

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De-Broglie Broglie Hypothesis

Proof: $E = h\nu$ and $E = mc^2 \implies h\nu = mc^2 \implies mc = \frac{h\nu}{c}$.

$$\therefore \quad p = mc = \frac{h\nu}{c} = \frac{h}{\lambda} \qquad (\because c = \nu\lambda)$$

$$\therefore \lambda = \frac{h}{p}.$$

Special cases:

- For a particle moving with non-relativistic velocity v, momentum $p = mv$,

$$\therefore \lambda = \frac{h}{mv}.$$

[Note: for relativistic velocity i.e., $v \to c$, $m = \frac{m_0}{\sqrt{1-v^2/c^2}}$.]

- Kinetic energy $E_K = \frac{1}{2}mv^2 = \frac{p^2}{2m} \implies p = \sqrt{2mE_K}$

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

De-Broglie Broglie Hypothesis

- If a charged particle is accelerated through a potential difference of V volt, then $E_K = qV$

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

- For case of electron,

$$\therefore \lambda = \frac{h}{\sqrt{2meV}} = \sqrt{\frac{150}{V}}\mathring{A}$$

- If a material particle is in thermal equilibrium at an absolute temperature T, then $E_K = \frac{3}{2}kT$,

$$\therefore \lambda = \frac{h}{\sqrt{3mkT}}$$

De-Broglie Broglie Hypothesis

Properties of Matter Waves or de-Broglie's Waves: From the expression $\lambda_m = \frac{h}{mv}$, it is clear that,

1. λ_m of heavy particle < λ_m of light weight particle.
2. λ_m of fast moving particle < λ_m of slow moving particle.
3. if $v = 0$ then $\lambda_m = \infty$, i.e., the matter waves are associated with only moving particles.
4. The matter wave can be generated by charged particles as well as by neutralized particles, i.e., matter wave does not depend on charge of particle.
5. The velocity of matter wave is not constant but depends on velocity of materials.
6. Matter waves are not EMWs.

De-Broglie Broglie Hypothesis

Q. Why matter waves are not EMW?

Ans. Because,

a. The matter waves are associated with only moving particles, irrespective of whether the particle is charged or not. Whereas EMWs are produced by only accelerated charges particles.

b. The velocity of matter waves is depends on the velocity of material particles but velocity of EMW is constant for a given medium.

De-Broglie Broglie Hypothesis

Q. Prove that velocity of matter wave is greater than the velocity of light.

Ans. From de-Broglie concept,

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

The energy of particle is

$$E = h\nu \quad \Longrightarrow \nu = \frac{E}{h}.$$

But from mass-energy relationship $E = mc^2$

$$\therefore \quad \nu = \frac{mc^2}{h}$$

We know that $c = \nu\lambda$

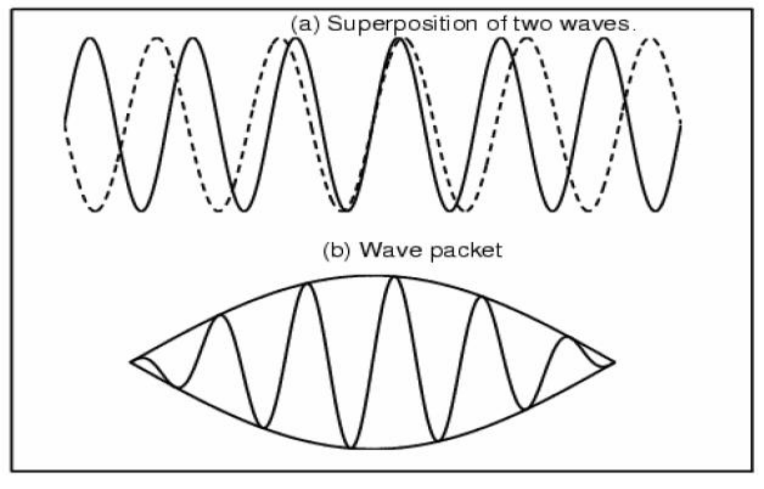
The de-Broglie wave velocity v_p is given as,

$$\begin{aligned} v_p &= \nu\lambda \\ &= \left(\frac{mc^2}{h}\right)\left(\frac{h}{mv}\right) \\ v_p &= \frac{c^2}{v}. \end{aligned}$$

Because $v < c$ always, hence *the matter wave always travels faster than light.*

Concept of wave-packet

Phase Velocity v_p ***& group velocity*** v_g: Consider two progressive waves, whose amplitude is same but angular frequency and propagation constant differs by $\Delta\omega$ and Δk respectively. Such wave can be written as,



$$y_1 = A\cos(\omega t - kx)$$
$$y_2 = A\cos[(\omega+\Delta\omega)t - (k+\Delta k)x]$$

According to principle of superposition,

$$\begin{aligned} Y &= y_1 + y_2 \\ &= A\left[\cos(\omega t - kx) + \cos[(\omega+\Delta\omega)t - (k+\Delta k)x]\right] \\ &= 2A\cos\left[\frac{(2\omega+\Delta\omega)t - (2k+\Delta k)x}{2}\right]\cos\left[\frac{\Delta\omega t - \Delta k x}{2}\right] \\ &\qquad \left[\because \cos A + \cos B = 2\cos\left(\frac{A+B}{2}\right)\cos\left(\frac{A-B}{2}\right)\right] \\ &= \underbrace{2A\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right)}_{amplitude}\cos(\underbrace{\omega t - kx}_{phase}) \end{aligned}$$

Concept of wave-packet

where $2\omega \approx 2\omega + \Delta\omega$ and $2k \approx 2k + \Delta k$. ω and k are mean angular frequency and mean propagation constant respectively.

For phase of the wave to be constant

$$\omega t - kx = \text{Constant}$$

$\therefore$ Wave velocity $\quad v_p = \frac{dx}{dt} = \frac{\omega}{k}$

Now for the amplitude of wave packet to be constant,

$$\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x = \text{constant}.$$

Hence the group velocity

$$v_g = \frac{dx}{dt} = \frac{\Delta\omega/2}{\Delta k/2} = \frac{\Delta\omega}{\Delta k}$$
$$= \lim_{\omega_1 \to \omega_2} \frac{\Delta\omega}{\Delta k} = \frac{d\omega}{dk}.$$

Concept of wave-packet

Relationship between group velocity v_g and phase velocity v_p:

$$\text{Wave velocity} \quad v_p = \frac{\omega}{k} \quad \Rightarrow \quad \omega = kv_p.$$

$$\text{Group velocity} \quad v_g = \frac{d\omega}{dk} = v_p + k\frac{dv_p}{dk} = v_p + \left(\frac{2\pi}{\lambda}\right)\frac{dv_p}{d\left(\frac{2\pi}{\lambda}\right)}$$
$$= v_p - \lambda\frac{dv_p}{d\lambda}.$$

Case I: In the non-dispersive medium, i.e., $dv_p/d\lambda = 0$, then $v_g = v_p$. For example, EMW propagation in vacuum.

Case II: In the dispersive medium,

1. If $dv_p/d\lambda = +ve$ then $v_g < v_p$. For example, EMW propagation in dielectric substance.
2. If $dv_p/d\lambda = -ve$ then $v_g > v_p$. For example, propagation in electric conductors.

Heisenberg's Uncertainty Principle, 1927

Statement: "It is impossible to determine the exact position and momentum of a particle simultaneously."

Proof: As per de-Broglie hypothesis, any moving particle is surrounded by packet of matter waves. See the figure (4). Now let consider this wave packet is formed due to superposition of two sinusoidal waves of different angular frequencies ω_1 & ω_2 and propagation constant k_1 & k_2 traveling along X-axis. The equations are,

$$\psi_1 = A\sin(\omega_1 t - k_1 x)$$
$$\psi_2 = A\sin(\omega_2 t - k_2 x)$$

Using superpostion principle,

$$\begin{aligned}\psi = \psi_1 + \psi_2 &= A\sin(\omega_1 t - k_1 x) + A\sin(\omega_2 t - k_2 x)\\ &= 2A\cos\left(\frac{\delta\omega}{2}t - \frac{\delta k}{2}x\right)\sin(\omega t - kx),\end{aligned}$$

where, $\omega = \dfrac{\omega_1 + \omega_2}{2}$, $k = \dfrac{k_1 + k_2}{2}$, $\delta\omega = \omega_1 - \omega_2$, and $\delta k = k_1 - k_2$.

Heisenberg's Uncertainty Principle, 1927

The error in the measurement of the position of the particle is equal to the distance between two nodes. These nodes are formed when $\cos\left(\frac{\delta\omega}{2}t - \frac{\delta k}{2}x\right) = 0$, i.e., $\left(\frac{\delta\omega}{2}t - \frac{\delta k}{2}x\right) = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \cdots$.

Let x_1 and x_2 are the position of any two successive nodes at any time t, then

$$\frac{\delta\omega}{2}t - \frac{\delta k}{2}x_1 = (2n+1)\frac{\pi}{2}$$
$$\text{and} \quad \frac{\delta\omega}{2}t - \frac{\delta k}{2}x_2 = (2n+3)\frac{\pi}{2}$$

on substraction,

$$\Longrightarrow \quad \frac{\delta k}{2}(x_2 - x_1) = \pi$$
$$\Longrightarrow \quad \Delta x = x_2 - x_1 = \frac{2\pi}{\delta k}$$
$$\Longrightarrow \quad \Delta x = \frac{2\pi}{\delta k} = \frac{2\pi}{\Delta\left(\frac{2\pi}{\lambda}\right)} = \frac{1}{\Delta\left(\frac{p}{h}\right)} = \frac{1}{\Delta p}$$
$$\Longrightarrow \quad \Delta x.\Delta p = h$$
$$\Longrightarrow \quad \Delta x.\Delta p \geq \hbar \ \left(= \frac{h}{2\pi}\right) \qquad \Longrightarrow \quad \boxed{\Delta x.\Delta p \geq \hbar}$$

Heisenberg's Uncertainty Principle, 1927

7.1 Energy and time uncertainty principle

We know that group velocity v_g is equal to particle velocity v_x. Let the wave packet moves Δx distance in Δt time. Since Δx is the uncertainty in the x-coordinate and Δt is the uncertainty in time, hence

$$v_g = \frac{\Delta x}{\Delta t} \qquad \Longrightarrow \qquad \Delta t = \frac{\Delta x}{v_g}. \tag{11}$$

$$\text{As energy} \quad E \equiv E(p_x)$$

$$\Delta E = \frac{\partial E}{\partial p_x}.\Delta p_x.$$

$$\text{But} \qquad \frac{\partial E}{\partial p_x} = v_x = v_g \qquad [\because\; E = \frac{1}{2}mv^2 \quad \longrightarrow \quad \frac{\partial E}{\partial v} = \frac{1}{2}2mv \quad \longrightarrow \quad \frac{\partial E}{\partial p} = v.]$$

$$\therefore \quad \Delta E = v_g.\Delta p_x \tag{12}$$

Using Eqs (11) and (12),

$$\Delta E.\Delta t = v_g.\Delta p_x.\frac{\Delta x}{v_g} = \Delta p_x.\Delta x \geq \hbar \qquad \text{[Using Heisenberg's uncertainty principle]}$$

$$\Longrightarrow \qquad \boxed{\Delta E.\Delta t = \hbar}$$

Applications of HUP (Non-existence of e in nucleus)

Since size of nucleus $= 10^{-14}m$, hence uncertainty in position inside the nucleus $= 2 \times 10^{-14}m$.

From Heisenberg's uncertainty principle,

$$\Delta p_x = \frac{\hbar}{\Delta x} = \frac{1.055 \times 10^{-14} J - sec}{2 \times 10^{-14}} m = 5.275 \times 10^{-21} Kg - m/s.$$

Since the magnitude of momentum is relativistic compare to the mass of the electron, then using relativistic mass formula for energy of electron,

$$E^2 = p^2c^2 + m_0^2c^4$$

$$E^2 = p^2c^2 \qquad [\because \quad m_0^2c^4 = 0.511MeV \ll p^2c^2]$$

$$E = pc = (5.275 \times 10^{-21}) \times (3 \times 10^8) J$$

$$= \frac{(5.275 \times 10^{-21}) \times (3 \times 10^8)}{1.6 \times 10^{-19}} eV = 10Mev.$$

Thus if the electron resides in the nucleus, it should have an energy of the order of $10MeV$. However, electrons emitted during β-decay have energies of the order of $3MeV$. Hence we conclude that electron do not reside in the nucleus.

Wave-function

8 The wave function ‘Ψ’

The wave function describes the wave properties of the moving particle. It is denoted by ‘Ψ’and is complex in nature, i.e., $\Psi = a + ib$, where a and b are real numbers.

8.1 Properties or physical significance of wave function

1. Ψ must be continues and single values everywhere.

2. $\frac{\partial\Psi}{\partial x}, \frac{\partial\Psi}{\partial y}, \frac{\partial\Psi}{\partial z}$ also must be continues and single values everywhere.

3. Ψ must be normalized, i.e., $\Psi = 0$ as $x \to \pm\infty$, $y \to \pm\infty$, $z \to \pm\infty$, i.e.,

$$\int_{-\infty}^{\infty} |\Psi|^2 \mathrm{d}V = 1.$$

Wave-function

4. $|\Psi|^2 = \Psi\Psi^*$ defines probability density and is at any particular place and time is proportional to the probability of finding the particle at that place on that time.

$$\text{Probability density} \qquad |\Psi|^2 = \Psi\Psi^*.$$

5. Probability $\quad P_{x_1x_2} = \int\limits_{x_1}^{x_2} |\Psi|^2 \mathrm{d}x.$

6. The expectation values: It is defined as,

   Position expectation values,

$$\langle x \rangle = \frac{\int\limits_{-\infty}^{\infty} x|\Psi|^2 \mathrm{d}x}{\int\limits_{-\infty}^{\infty} |\Psi|^2 \mathrm{d}x} = \int\limits_{-\infty}^{\infty} x|\Psi|^2 \mathrm{d}x. \qquad \text{[for normalized function.]}$$

Energy expectation values,

$$\langle E \rangle = \frac{\int\limits_{-\infty}^{\infty} E|\Psi|^2 \mathrm{d}x}{\int\limits_{-\infty}^{\infty} |\Psi|^2 \mathrm{d}x} = \int\limits_{-\infty}^{\infty} E|\Psi|^2 \mathrm{d}x. \qquad \text{[for normalized function.]}$$