INTRODUCTION TO QUANTUM MECHANICS

(**Module - II – Syllabus: Principles of Quantum Mechanics:** Introduction – de Broglie's hypothesis for matter waves - Davison and Germer's experiment - Schrödinger's one dimensional wave equation (time independent) - significance of wave function – Fermi Dirac distribution and effect of temperature (qualitative treatment).

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Introduction: Classical mechanics is useful to explain the motion of macroscopic particles, but it failed to explain the Photoelectric effect, Compton Effect, and black body radiation. Max Planck proposed quantum theory at the beginning of the 20^{th} century. Based on the ideas of quantum theory, a new mechanics called quantum mechanics was developed in 1925.

Waves and Particles:

A wave is simply defined as spreading out of the disturbance through the medium in all directions uniformly. It is not possible to say the wave position since physically it can't be seen. The characteristics of a wave are wavelength (λ), frequency (ν), wave velocity (ω), amplitude (A), phase (φ), intensity (I), …..

A particle has a definite mass and occupies a particular point. When the force is applied to it, it moves in the force direction and it can be physically seen. Characteristics of particles are mass (m), velocity (v), momentum (p), energy (E), ….

As per the above facts, radiation exhibits a dual nature. The experiments' Photoelectric effect and Compton effect say that the radiation exhibits particle nature, whereas experiments like interference and diffraction say it exhibits wave nature.

Hence it can be concluded that radiation is exhibiting dual nature. i.e. wave nature as well as particle nature. But it is not possible to exhibit both wave nature and particle nature at a time.

** de-Broglie's Hypothesis of matter waves:

In 1924, Louis de-Broglie proposed the dual nature of matter. According to his hypothesis, when the particle is accelerated, then it will spread like a wave with a certain wavelength. He has given a mathematical equation to support the hypothesis. *Electromagnetic waves behave like particles, and particles like electrons will behave like waves called matter waves.*

We have Planck's theory of radiation, the energy of the photon is $E = h\nu$ (wave aspect)

$$E = \frac{hc}{\lambda} \quad \text{------ (1)} \qquad (\because c = \nu\lambda)$$

where 'c' is the velocity of light, 'λ' is the wavelength, and 'h' is Planck's constant

From Einstein's mass-energy relation $E = mc^2$ ------ (2) (particle aspect)

where 'm' is the mass of the photon

from Eq. (1) & (2) $mc^2 = \frac{hc}{\lambda}$

$$\lambda = \frac{h}{mc} \rightarrow \lambda = \frac{h}{p}$$ where 'p' is momentum of the photon.

Applying de-Broglie's hypothesis to particle: Let an electron of charge 'e', mass 'm' moving with velocity 'v' in presence of potential 'V' then the wavelength associated with the electron is

$$\lambda = \frac{h}{mv} \rightarrow \lambda = \frac{h}{p} \quad \text{------ (3)}$$

when an electron is in motion, then its kinetic energy is $\frac{1}{2}mv^2$

we have the energy of the electron (E) in terms of potential is eV

$$\therefore eV = \frac{1}{2}mv^2$$

multiplying above Eq. with ‘m’

$$m\,e\,V = \frac{1}{2}m^2v^2$$

$$m\,e\,V = \frac{p^2}{2}$$

$$p = \sqrt{2meV} \qquad \text{------ (4)}$$

substituting Eq. (4) in Eq. (3)

$$\lambda = \frac{h}{\sqrt{2meV}} \quad \text{or} \quad \frac{h}{\sqrt{2mE}} \qquad \text{------ (5)}$$

here ‘h’ is Planck’s constant = 6.625×10^{-34} JS

‘m’ is mass of electron = 9.1×10^{-31} kg

‘e’ is charge of electron = 1.6×10^{-19} Coulombs

on substituting the above values in Eq. (5), we get $\lambda = \frac{12.26 \times 10^{-10}}{\sqrt{V}} \rightarrow$ $\boxed{\lambda = \frac{12.26}{\sqrt{V}}\ \text{Å}}$

It shows the wavelength associated with an electron in the presence of potential difference ‘V’.

Properties of matter waves:

1. de-Broglie’s waves are not electromagnetic waves, they are called pilot waves.
2. Waves can’t be observed.
3. Lighter is the particle, and greater is the wavelength.
4. Smaller the velocity of the particle, the greater will be the wavelength.
5. V = 0 then $\lambda = \infty$, this shows that matter wave is associated with moving particles.
6. Matter waves travel faster than the velocity of light. $\omega = \frac{c^2}{v}$
7. Whether the particle is charged or not, a matter wave is associated with it.
8. No single phenomenon exhibits both particle nature & wave nature at a time.

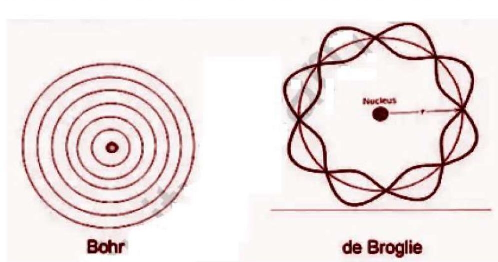
Note: According to Bohr’s postulates, electrons revolve around the nucleus, and the energy of electrons is quantized.

Angular momentum (L) of moving electron is $mvr = \frac{nh}{2\pi}$

$2\pi r = \frac{nh}{mv} \quad \rightarrow \quad 2\pi r = n\lambda$

i.e. circumference of the electron orbit ($2\pi r$) equal to

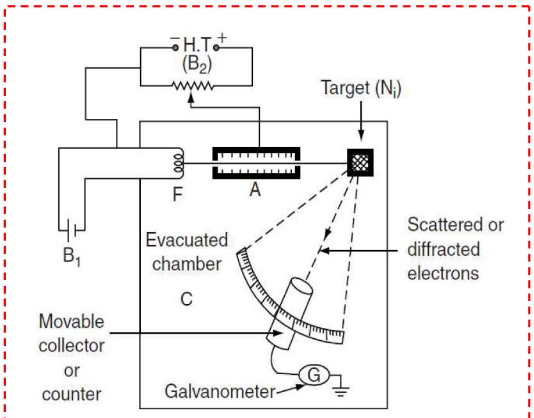
‘n’ times of ‘λ’ associated with the electron.



** Davison and Germer's experiment:

In general, waves exhibit a diffraction phenomenon. If the wavelength of the wave is comparable to slight width then diffraction occurred. If de Broglie's hypothesis is valid, then matter waves should exhibit a diffraction effect.

The experimental arrangement is shown in Fig. The apparatus consists of an evacuated chamber 'C'. Inside this chamber, electrons are produced by heating the filament 'F' with a low-voltage battery (B_1). The emitted electrons are attracted by an anode 'A' connected to an H.T. variable voltage source. A fine beam of electrons is coming from the filament 'F' and allowed to the incident on a nickel crystal (Ni) (the crystal can be rotated about an axis). As a result, these electrons were scattered by the nickel crystal. The intensities of the scattered electrons are measured with the help of a detector/counter. This detector is moving along a semicircular scale (ranging from 20° to 90° w.r.t. the incident beam). The accelerating potential of the anode is varied in the range of 30 to 600 V. The deflection in the galvanometer is proportional to the number of scattered electrons received by the counter.



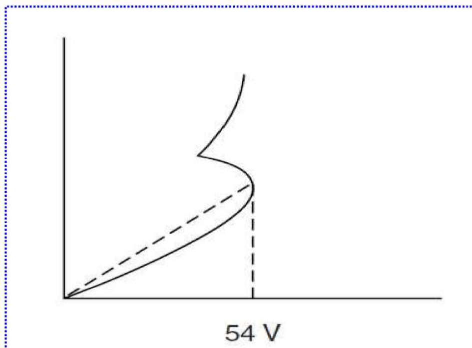


Fig. Polar curve corresponding to 54 V

A polar graph was plotted between the detector current and the angles of scattered electrons with the incident beam. It was found that the graph remains smooth up to the accelerated voltage of 44 V. When the accelerating voltage is 44 V, then a hump was observed on the curve and this becomes more intense at 54 V, later this hump diminishes above 68 V. *In this experiment, it was observed that the intensity of scattered electrons was maximum at an angle of 50° w.r.t. ident beam, when the accelerating voltage is 54 V in the case of nickel crystal.*

From the XRD studies, the angle between the incident and diffracted electron beam makes an angle [θ] of 65°. By substituting this θ in Bragg's equation, $2d \sin\theta = n\lambda$. where d = interplanar spacing, n = order of diffraction, and λ is the wavelength. The 'd' value for the nickel crystal is 0.091 nm.

$$\therefore 2d \sin\theta = n\lambda \rightarrow 2 \times (0.091\times10^{-9}) \times \sin 65° = 1\lambda \rightarrow \lambda = 0.165 \text{ nm}.$$

The Wavelength of the waves associated with the incident beam of electrons using de Broglie's equation is

$$\lambda = \frac{12.26 \text{ x } 10^{-10}}{\sqrt{V}} = \frac{12.26 \text{ x } 10^{-10}}{\sqrt{54}}$$

$\lambda = 0.166$ nm

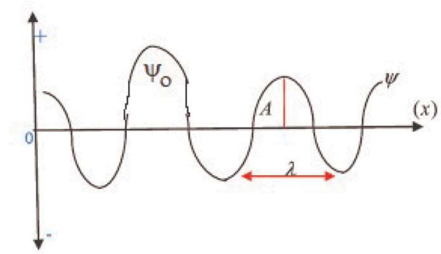
This value is in good agreement with the experimental value. Hence Davison and Germer's experiment proves the de Broglie hypothesis of the wave nature of moving particles.

** Schrödinger time independent wave equation:

Based on de Broglie's idea of matter waves, Schrödinger in 1926 developed a wave equation for the moving particles. According to him, let a particle of mass 'm' moving with velocity 'v' associated with a group of waves (along the x-axis).

Let us consider a simple form of progressive wave is $\psi = \psi_0$ Sin (ωt - kx) ------ (1)

where ψ be the wave function of the particle, ψ_0 is amplitude



Differentiating Eq. (1) w.r.t. 'x' twice

$$\frac{\partial \psi}{\partial x} = \psi_0 \text{Cos}(\omega t - kx)(-k)$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\psi_0 \text{Sin}(\omega t - kx)(k^2)$$

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2\psi \qquad [\because \text{from Eq.1, } \psi = \psi_0 \text{Sin}(\omega t - kx)]$$

$$\frac{\partial^2 \psi}{\partial x^2} + k^2\psi = 0$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{4\pi^2}{\lambda^2}\psi = 0 \qquad \text{------ (2)}$$

where 'k' is the propagation constant, $k = \frac{2\pi}{\lambda}$

The above equation is a differential form of the classical wave equation.

We have de Broglie's wavelength (λ) = $\frac{h}{mv}$, substituting this equation in Eq. (2)

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{4\pi^2 m^2 v^2}{h^2}\psi = 0 \qquad \text{------ (3)}$$

The total energy (E) of the particle is the sum of KE & PE

E = KE + PE → E = K + V ------ (4)

$KE = K = \frac{1}{2}mv^2$

$2K = mv^2$

$$2Km = m^2v^2 \quad \text{------ (5)}$$ (multiplying above equation with 'm')

$$2(E - V)m = m^2v^2$$ [∵from Eq.(4) → K = E-V]

Substituting the above equation in Eq.(3)

$$\frac{\partial^2\psi}{\partial x^2} + \frac{8\pi^2 m(E-V)}{h^2}\psi = 0$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m(E-V)}{\hbar^2}\psi = 0 \quad \text{------ (6)}$$ where $\hbar = \frac{h}{2\pi}$

The above equation represents one dimensional Schrödinger time independent wave equation.

When it is extended to a 3-dimensional wave

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{2m(E-V)}{\hbar^2}\psi = 0 \quad \text{------ (7)}$$

Laplacian operator

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Eq.(7) becomes $$\boxed{\nabla^2\psi + \frac{2m(E-V)}{\hbar^2}\psi = 0}$$

This is a Schrödinger wave equation and the time factor doesn't appear.

Hence it is time independent wave equation.

** Significance of wave function (ψ):

1. Wave function gives the information about the particle behavior statistically.
2. Wave function (ψ) is a mathematical tool used in quantum mechanics.
3. ψ is a complex quantity and individually it does not have any meaning.
4. $|\psi^2| = \psi^*\psi$ is real and positive, it has physical meaning.
5. For a given volume it is given by $|\psi^2|dv$
6. $|\psi|^2$represents probability density.
7. It can tell the probability of the position of the particle at a time, but it can not predict the exact location of the particle at that time.

** Fermi-Dirac distribution and effect of temperature: (qualitative treatment)

The electron is an indistinguishable particle hence it is called a Fermi particle. In absence of an electric field electrons present in metal move randomly and behaviors as electron gas. According to quantum theory at absolute zero temperature (0 K) the free electrons occupy in the energy levels without any vacancy. This can be understood by dropping the free electrons of a metal one by one into a potential well. The 1st electron would occupy the lowest available energy (E_0), if the next (2nd) electron dropped into the well, it also occupy in same energy level. The 3rd electron dropped into the potential well it occupies in the next higher level i.e E_1 ($E_1 > E_0$) and so on. This process continued based on the *Pouli's exclusives principle*. If metal consists of an 'N' number of electrons, they will distribute in ($^N/_2$) energy levels and the higher level will be empty. (Fig.i)

The highest energy level occupied by an electron at absolute zero (0 K) is known as the ***Fermi energy level*** and the corresponding energy is known as Fermi energy (E_F). As the temperature of metals increases from 0 K to T K, the electron present below E_F regions takes thermal energy and moved to a higher energy level, whereas electrons present in the lower energy level will not take thermal energy because they will not find vacant electron states.

The Fermi-Dirac distribution function is given by

$$F(E) = \frac{1}{1 + \exp\left[\frac{E - E_F}{KT}\right]}$$

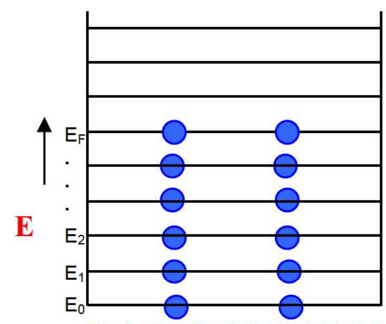


Fig.i Distribution of electrons in various energy levels at 0 K

Where F(E) is the probability of occupation of an electron in a particular energy

K is Boltzmann constant (1.38×10^{-23} JK^{-1})

At temperature T > 0 K

1) for $E < E_F$, $E - E_F$ = - Ve then F (E) ≈ 1

2) for $E > E_F$, $E - E_F$ = + Ve then F (E) ≈ 0

3) for $E = E_F$, $E - E_F$ = 0 then F (E) = ½

It means, at finite temperature the probability occupancy of the Fermi level is ½

At temperature T = 0 K, for $E < E_F$, F (E) ≈ 1 and for $E > E_F$ F(E) ≈ 0

From Fig. ii, it is clear that bellow the E_F has filled electron and above it is empty. As the temperature increases to T_1 K, the step becomes curved. Further increase in temperature to T_2 K, T_3 K the tails of curve increases. This indicates that more and more electrons occupy higher energy states with an increase in temperature.

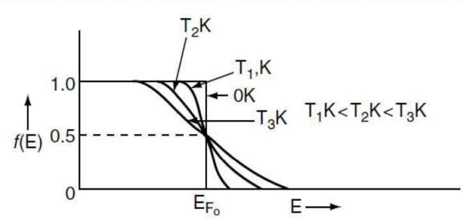


Fig.ii

At non-zero temperature all these curves pass through a point whose F(E) = ½ at $E = E_F$, which means E_F lies halfway between the filled and empty state.

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