MODULE - 1

MODERN PHYSICS

Dual nature of matter

The photoelectric effect and the Compton scattering conclusively established the particle behavior of light. The phenomena of interference, diffraction and polarization give exclusive evidence for the wave behavior of light. On one hand, light resembles a collection of particles having energy E and momentum p and on the other hand, it is regarded as a continuous wave of frequency (γ). Either of these separate pictures is not in a position to explain all the experimental results and hence, we have to conclude that light behaves as an advancing wave in some phenomenon and it behaves as a flux of particles in some other phenomena. Therefore, we say that light exhibits ***wave-particle duality***.

de Broglie's hypothesis

We know that the phenomenon such as interference, diffraction, polarization etc. can be explained only with the help of wave theory of light. While phenomenon such as photoelectric effect, Compton effect, spectrum of blackbody radiation can be explained only with the help of Quantum theory of radiation. Thus radiation is assumed to exhibit dual nature. i.e. both the particle and wave nature. In 1924, **Louis de-Broglie** made a bold hypothesis, which can be stated as follows

"If radiation which is basically a wave can exhibit particle nature under certain circumstances, and since nature likes symmetry, then entities which exhibit particle nature ordinarily, should also exhibit wave nature under suitable circumstances."

Thus according to De-Broglie's hypothesis, there is wave associated with the moving particle. Such waves are called **Matter waves** and wavelength of the wave associated with the particle is called **De-Broglie wavelength.**

Expression for de Broglie wavelength:

As a photon travels with the velocity c, we can express its momentum as,

$$p = \frac{E}{c}$$

$$p = \frac{h\gamma}{c}$$

$$p = \frac{h}{\lambda} \tag{10}$$

Thus, the wavelength λ and momentum *p* of a photon are related to each other through the expression

$$\lambda = \frac{h}{p} \tag{11}$$

De Broglie proposed that the relation (11) between the momentum and the wavelength of a photon is a universal one and must be applicable to photons and material particles as well.

Now, let us consider a moving particle. A particle of mass *m* moving with a velocity *v* carries a momentum $p = mv$ and it must be associated with a wave of wavelength

$$\lambda = \frac{h}{mv} \tag{12}$$

Relation (12) is known as ***de Broglie equation*** and the wavelength λ is called the ***de Broglie wavelength***.

De-Broglie wavelength associated with an accelerated charged particle:

If a charged particle, say an electron is accelerated by a potential difference of *V* volts, then its kinetic energy is given by

$$E_K = eV.$$

$$\text{or } \frac{1}{2}mv^2 = eV$$

$$v = \sqrt{\frac{2eV}{m}}$$

Then the electron wavelength is given by,

$$\lambda = \frac{h}{mv} = \frac{h}{m}\sqrt{\frac{m}{2eV}}$$

$$\text{Thus, } \lambda = \frac{h}{\sqrt{2meV}} \tag{13}$$

By substituting the values of constants h, m and e in eq. (13), we get,

$$\lambda = \frac{6.626x10^{-34}}{\sqrt{2x(9.11x10^{-31})x(1.602x10^{-19}V)}} = \frac{1.226x10^{-9}}{\sqrt{V}} m$$

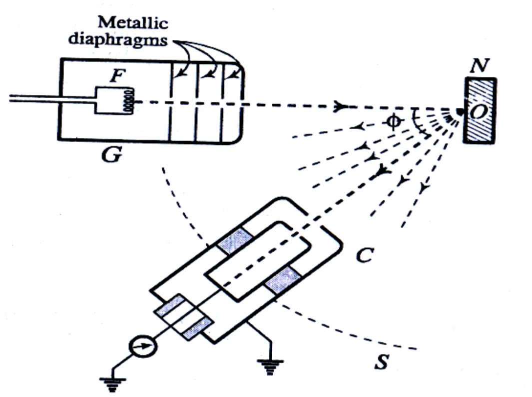
$$\text{or } \boxed{\lambda = \frac{1.226}{\sqrt{V}} nm}$$

Davisson-Germer's experiment:

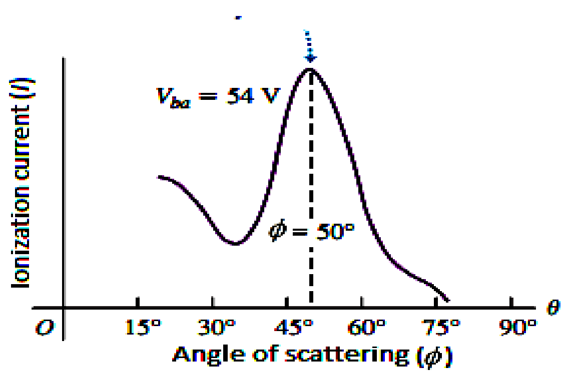
Davisson and Germer were studying the phenomenon of scattering of electrons from material targets and they observed *diffraction of electrons* in a crystal of nickel, similar to *X-ray waves undergoing diffraction* in crystals, thus proving the wave behavior of electrons.

The experimental apparatus is as shown in the above fig. consists of an electron gun G, which produces a narrow and collimated beam of electrons accelerated to known potential V. a solid nickel crystal used as a target mounted on a rotatable stand and an ionization chamber (detector) C which is connected to a galvanometer to collect and measure the current due to the scattered electrons.

Electron beam is made to strike the nickel crystal C. Electrons scattered from the crystal is collected by the ionization chamber at various scattering angles ϕ and the corresponding value of ionization current I is noted. Experiment is repeated for various accelerating potentials V. A graph representing ϕ and I for different values of V is plotted. The graph obtained is shown in the fig.



DAVISSON AND GERMER'S EXPERIMENTAL ARRANGEMENT

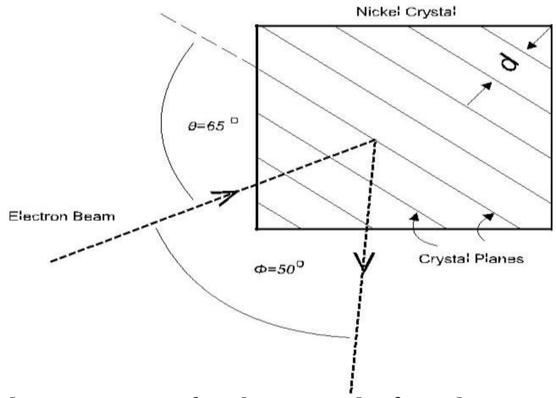


Initially, when accelerating potential was 40 V a smooth curve was obtained. When potential was increased to 44 V ionization current started to increase and reaches maximum for the accelerating potential of 54 V. The scattering angle corresponding to the accelerating Potential 54 V when Ionization current became maximum was found to be $\phi = 50^0$.

Davisson and Germer interpreted the result as follows:

Electrons in the incident beam behave like waves. Thus when electrons strike the crystal they undergo Bragg's diffraction from the different planes of the crystal. The bump in the curve corresponds to constructive interference caused by the scattered electrons. According to Bragg's law the condition for constructive interference is given by

$$2d\sin\theta = n\lambda$$



where d = Interplanar spacing for the crystal, θ = glancing angle made by incident beam with the crystal plane, n=order and λ is wavelength of the wave. Thus, when bump in the curve is maximum, $\theta = 65^0$ (see fig of crystal), n=1 and for nickel crystal, d = 0.91 A^0. Thus, wavelength of the waves associated with the electrons is given by

$$\lambda = 2\times 0.91\times 10^{-10}\times Sin(65^0) = 1.65\times 10^{-10}\,m$$

According to de Broglie's hypothesis for an electron accelerated by potential difference of 54 V the de Broglie wavelength is given by

$$\lambda = \frac{12.26}{\sqrt{V}}A^o = \frac{1.226\times 10^{-9}}{\sqrt{54}} = 1.66\times 10^{-10}\,m$$

The experimentally determined value is in good agreement with the value calculated according to de Broglie's hypothesis. Thus Davisson and Germer experiment not only confirms the wave associated with moving particle it also verifies the de Broglie's hypothesis.

Phase velocity and Group velocity

Phase velocity (v_p)

The velocity with which a wave travels is called phase velocity and is also called wave velocity. If a point is marked on the wave representing the phase of the particle then the velocity with which the phase propagates from one point to another is called phase velocity. It is given by

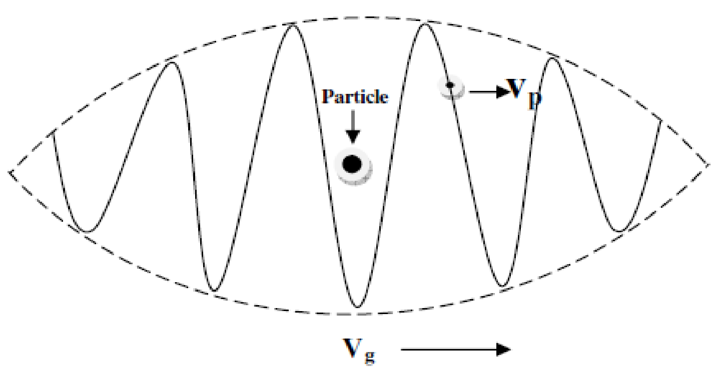
$v_p = \frac{\omega}{k}$ Where 'ω' is the angular frequency and 'k' is wave number. Substituting for $\omega = 2\pi\nu$ and $k = \frac{2\pi}{\lambda}$. We get $v_p = \nu\lambda$,

Therefore $v_p = \frac{h\nu}{\frac{h}{\lambda}} = \frac{E}{p}$ Where 'E' is the energy and 'p' is momentum

$v_p = \frac{mc^2}{mv} = \frac{c^2}{v}$ Where 'c' is the velocity of light and 'v' is the velocity of the article.

From the above expression it is evident that the phase velocity is not only greater than the particle velocity it is also greater than the velocity of light. Hence there is no physical meaning for phase velocity of matter waves.

Group velocity (v_g)



Since the velocity of matter waves must be equal to that of the particle velocity and since no physical can be associated with phase velocity the concept of group velocity is introduced. Matter wave can be considered as a resultant wave due to the superposition of many component waves whose velocities differ slightly. Thus a wave group or wave packet is formed. The velocity with which the wave group travels is called group velocity which is same as particle velocity. It is denoted by v_g.

Properties of Matter waves

The following are the properties associated with the matter waves

1) Matter waves are associated only with particles in motion
2) They are not electromagnetic in nature
3) Group velocity is associated with matter waves
4) The phase velocity has no physical meaning for matter waves
5) The amplitude of the matter wave at a given point is associated with the probability of finding the particle at that point.
6) The wavelength of matter waves is given by $\lambda = \frac{h}{p}$

WAVE MECHANICS

Heisenberg's Uncertainty Principle

Statement: "The simultaneous determination of the exact position and momentum of a moving particle is impossible"

Explanation: According to this principle if Δx is the error involved in the measurement of position and Δp is the error involved in the measurement of momentum during their simultaneous measurement, then the product of the corresponding uncertainties is given by

$$\Delta x \times \Delta p \geq \frac{h}{4\pi} \quad similarly \;\; \Delta E \times \Delta t \geq \frac{h}{4\pi}$$

The product of the errors is of the order of Planck's constant. If one quantity is measured with high accuracy then the simultaneous measurement of the other quantity becomes less accurate.

Physical significance: According to Newtonian physics the simultaneous measurement of position and momentum are "exact". But the existence of matter waves induces serious problems due to the limit to accuracy associated with the simultaneous measurement. Hence the "Exactness" in Newtonian physics is replaced by "Probability" in quantum mechanics.

Suggested reading: Principle of complementarity and Schrodinger's cat.

Application of Heisenberg's uncertainty principle

Non-existence of the electron in the nucleus: Beta rays are emitted by the nucleus. When it was first observed it was believed that electrons exist inside the nucleus and are emitted at certain instant. If the electron can exist inside the atomic nucleus then uncertainty in its position must not exceed the diameter of the nucleus. The diameter of the nucleus is of the order of 10^{-14}.

Applying Heisenberg's uncertainty principle for an electron expected to be inside the nucleus we get

$$\Delta x \times \Delta p \geq \frac{h}{4\pi}$$

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

Substituting for Δx and h we get

$\Rightarrow \Delta p \geq \frac{h}{4\pi\, \Delta x} \geq \frac{6.625 \times 10^{-34}}{4 \times 3.142 \times 10^{-14}} \geq 0.52 \times 10^{-20}\, N\, s$ is the uncertainty in the measurement of momentum. Thus the momentum of the electron must be at least equal to the uncertainty in the momentum. Therefore $p_x = 0.52 \times 10^{-20}\ N\ s$

The energy of the electron is given by relativistic equation $E = p_x\, c$

Where **c = 3x10^{8} m/s** is the velocity of light. Substituting the values, the energy of the electron expected to be inside the nucleus is given by

E=1.5x10^{-12} J ~ 9.7 MeV

According to experiments, the energy associated with the Beta ray emission is around 3 MeV which is much lesser than the energy of the electron expected to be inside the nucleus. Hence electrons do not exist inside the nucleus.

Wave Function

According to the Deborglie's Hypothesis the relation between momentum and wavelength is found to be experimentally valid for both photons and particles. The quanta of matter or radiation can be represented in agreement with uncertainty principle by wave packets. Thus it suggests that concentrated bunches of waves might be used to describe localized particles and quanta of radiation. Hence we shall consider a wave function that depends on space (x, y and z) and time (t) and is denoted by ψ (psi). The wave function for a wave packet moving along +ve X axis is given by

$$\psi = \psi_0 e^{-i(\varpi t - kx)}$$

Time-Independent Schrödinger Wave Equation

The wave equation which has variations only with respect to position and describes the steady state is called Time-Independent Schrodinger wave equation.

Consider a particle of mass '**m**' moving with velocity 'v' along +ve X-axis. The deBroglie wave length '**λ**' is given by

$$\lambda = \frac{h}{mv} \quad ....(1)$$

The wave equation for one dimensional propagation of waves is given by

$$\frac{\partial^2\psi}{\partial x^2} = \frac{1}{\mathrm{v}^2}\frac{\partial^2\psi}{\partial t^2} \quad ....(2) \quad along\ +ve\ X-axis$$

$$Where\ '\mathrm{v}'\ is\ Wave\ Velocity$$

Here $\psi = \psi_0 e^{-i(\omega t - kx)}$ ....(3)

Where ψ_0 is the amplitude at the point of consideration **ω** is angular frequency and **k** is Wave Number.

Differentiating ψ twice with respect to time (t), we get

$$\frac{\partial^2\psi}{\partial t^2} = -\omega^2\psi_0 e^{-i(\omega t - kx)} \quad ....(4)$$

Substituting equation (4) in equation (2)

$$\frac{\partial^2\psi}{\partial x^2} = \frac{1}{\mathrm{v}^2}\left(-\omega^2\psi\right) = \frac{1}{(f\lambda)^2}(-2\pi f)^2\psi \quad Here\ \ f\ \ is\ the\ \ frequency\ of\ \ the\ wave\ \ and\ \lambda\ is\ the\ wavelength$$

$$\therefore \frac{\partial^2\psi}{\partial x^2} = -\left(\frac{4\pi^2}{\lambda^2}\right)\psi$$

$$\Rightarrow \frac{\partial^2\psi}{\partial x^2} + \left(\frac{4\pi^2}{\lambda^2}\right)\psi = 0$$

Substituting for λ from equation (1) we get

$$\frac{\partial^2\psi}{\partial x^2} + \left(\frac{4\pi^2}{\left(\frac{h}{mv}\right)^2}\right)\psi = 0$$

$$\frac{\partial^2\psi}{\partial x^2} + \left(\frac{4\pi^2}{h^2}\right)\frac{2\,m^2v^2}{2}\psi = 0$$

$$\frac{\partial^2\psi}{\partial x^2} + \left(\frac{8\pi^2 m}{h^2}\right)\frac{1}{2}mv^2\psi = 0 \quad ....(5)$$

The kinetic energy of the particle $\frac{1}{2}mv^2$ is given by

$$\frac{1}{2}mv^2 = E - V \quad here\ E\ \ is\ the\ Total\ Energy\ of\ the\ particle\ and\ V\ is\ the\ Potential\ Energy$$

Therefore equation (5) becomes

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

Generalizing the equation for three dimensions we get

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

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

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

Hence the Time-Independent Schrodinger Wave equation for three dimensions.

Physical significance of wave function (Physical Interpretation)

The wave function ψ just as itself has no direct physical meaning. It is more difficult to give a physical interpretation to the amplitude of the wave. The amplitude of the wave function ψ is certainly not like displacement in water wave or the pressure wave nor the waves in stretched string. It is a very different kind of wave. But the quantity, the squared Absolute amplitude gives the probability for finding the particle at given location in space and is referred to as probability density. It is given by

$$P(x) = |\psi|^2$$

Thus, in one dimension the probability of finding a particle in the width ‘dx’ of length ‘x’

$$P(x)\ dx = |\psi|^2\ dx$$

Similarly, for three dimension, the probability of finding a particle in a given small volume dV of volume V is given by

$$P\ dV = |\psi|^2\ dV \quad here\ dV = dx\ dy\ dz.$$

Here 'P' Probability of finding the particle at given location per unit volume and is called Probability Density.

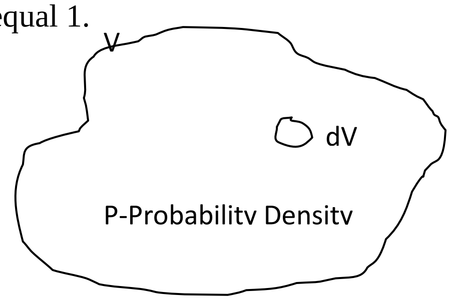
But since ψ is complex the probability density $|\psi|^2$ is given by

$$|\psi|^2 = \psi\psi^*$$

Where ψ* is the complex conjugate of ψ and the above product results in real number.

Normalization and Normalized wave function

Since the particle exists somewhere in volume V then the probability of finding the particle in the given volume V is equal 1.



Thus $$\int_0^V |\psi|^2 \; dV = 1 = \int_0^V P \; dV$$

If we are unable to locate the particle in volume V then the notion can be extended to the whole space with

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

But, normally, the value of the above integral will not be unity but contains an indefinite constant which can be determined along with sign using above considerations. The process is called normalization and the wave function which satisfies the above condition is called normalized wave function.

Eigen functions and Eigen values

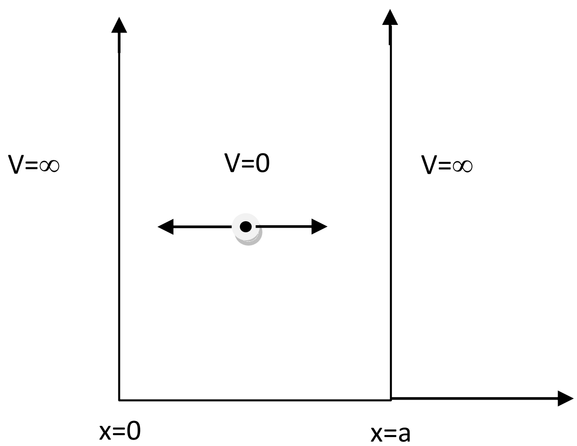
The Schrodinger wave equation is a second order differential equation. Thus solving the Schrodinger wave equation to a particular system we get many expressions for wave function (ψ). However, all wave functions are not acceptable. Only those wave functions which satisfy certain conditions are acceptable. Such wave functions are called Eigen functions for the system. The energy values corresponding to the Eigen functions are called Eigen values. The wave functions are acceptable if they satisfy the following conditions

1) ψ must be finite everywhere (not zero everywhere)
2) ψ must be single valued which implies that solution is unique for a given position in space
3) ψ and its first derivatives with respect to its variables must be continuous everywhere.

Applications of Schrödinger wave equation

Particle in a one dimensional box or one dimensional potential well of infinite height

Consider a particle of mass 'm' bouncing back and forth between the walls of one dimensional potential well. The particle is said to be under bound state. Let the motion of the particle be confined along the X-axis in between two infinitely hard walls at x=0 and x=a. Since the walls are infinitely hard, no energy is lost by the particle during the collision with walls and the total energy remains constant.



In between walls i.e. $0 < x < a$, the potential energy V=0.

Beyond the walls i.e. $x \le 0$ and $x \ge a$, the potential energy V=∞.

Beyond the walls

Since the particle is unable to penetrate the hard walls it exists only inside the potential well. Hence ψ=0 and the probability of finding the particle outside the potential well is also zero.

Inside the potential well

Since the potential inside the well is V=0, the Schrodinger wave equation is given by

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

$$\therefore \frac{\partial^2\psi}{\partial x^2} + \frac{8\pi^2 m E}{h^2}\,\psi = 0$$

$$\frac{\partial^2\psi}{\partial x^2}+k^2\ \psi=0 \quad ....(1) \quad \text{Here } k^2=\frac{8\pi^2 mE}{h^2} \quad ....(2)$$

For the given value of E, k is constant. The general solution for the equation (1) is given by

$\psi(x)=A\sin kx+B\cos kx$ ....(3) Where A and B are arbitrary constants. The values of these constants can be obtained by applying the boundary conditions

I) At x=0 , $\psi(x)=0$. Substituting the values in equation (3) we get

$$0=A\sin 0+B\cos 0$$
$$\therefore B=0$$
$$Hence\ \ equation(3)\ becomes\ \psi(x)=A\sin kx \quad ....(4)$$

II) At x=a, $\psi(x)=0$. Substituting the values in equation (4) we get

$$0=A\sin ka$$
$$Since\ \ A\neq 0\ (Otherwise\ no\ Solution),\ \ ka=n\pi \ \text{ Where n= 1, 2, 3,……}$$
$$\Rightarrow k=\frac{n\pi}{a} \ ....(5)$$

Thus the wave function becomes $\psi(x)=A\sin\frac{n\pi x}{a}$ ....(6)

Also substituting the value of 'k' from eq (5) into eq (2) we get

$$\left(\frac{n\pi}{a}\right)^2=\frac{8\pi^2 mE}{h^2} \quad \Rightarrow \quad E=\frac{n^2h^2}{8ma^2} \quad ....(7)$$ hence the energy **Eigen values**.

Thus substituting n=1 in the equation (7) we get

$E_1=\frac{h^2}{8ma^2}$ is the ground state energy of the particle and is also called zero point energy.

Hence $E_n=n^2E_1$ E_2 and E_3 are energies of the first and second excited states respectively and so on. Hence for a particle in the bound state, the energy values are discrete.

Normalization of wave function

The wave function for a particle in a box is given by equation (6)

$$\psi(x)=A\sin\frac{n\pi x}{a}$$

The value of the arbitrary constant '**A**' can be determined by the process of normalization. Since the particle has to exist somewhere inside the box we have

$$\int_0^a P(x)\,dx = \int_0^a |\psi(x)|^2 \; dx = 1$$ Substituting the wave function from equation (6)

$$\int_0^a A^2 \; \sin^2\left(\frac{n\pi\, x}{a}\right) dx = 1$$

Since $\sin^2\theta = \frac{1}{2}[1-\cos 2\theta]$ we have

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

Integrating the equation we get

$$\frac{A^2}{2}\left[x - \frac{a}{2n\pi}\sin\left(\frac{2\,\pi\, n\, x}{a}\right)\right]_0^a = 1$$ The second term takes the value zero for both the limits

$$\therefore \frac{A^2}{2}[a-0] = 1 \Rightarrow A = \sqrt{\frac{2}{a}}$$

Thus the **Eigen function** is given by

$$\psi_n(x) = \left[\sqrt{\frac{2}{a}}\right]\sin\frac{n\pi\, x}{a}$$

The wave functions and the probability densities for the first three values of '**n'** are as shown in fig

Thus for ground state (n=1) The probability of finding the particle at the walls is zero and at the centre (a/2) is maximum. The first excited state has three nodes and the second excited state has four nodes.