Wave Particle Dualism

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,

$$p = \frac{E}{c} = \frac{h\gamma}{c} = \frac{h}{\lambda} \tag{10}$$

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

$$\lambda = \frac{h}{p} \qquad (11)$$

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

$$\lambda = \frac{h}{mv} \qquad (12)$$

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,

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

$$\text{Thus, } \lambda = \frac{h}{\sqrt{2meV}} \qquad (13)$$

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

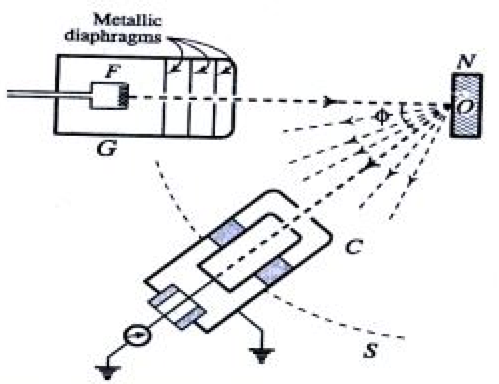
$$\lambda = \frac{6.626x10^{-34}}{\sqrt{2x\left(9.11x10^{-31}\right)x\left(1.602x10^{-19}V\right)}} = \frac{1.226x10^{-9}}{\sqrt{V}}m$$

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

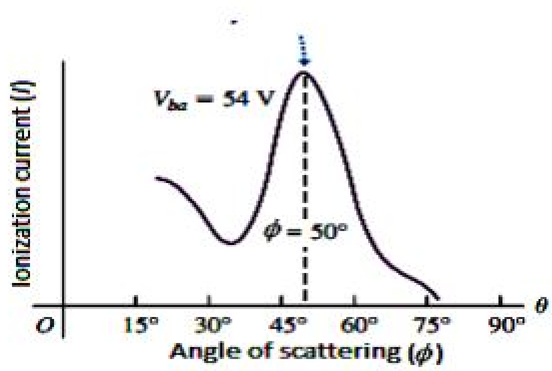
Davisson-Germer's experiment:

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



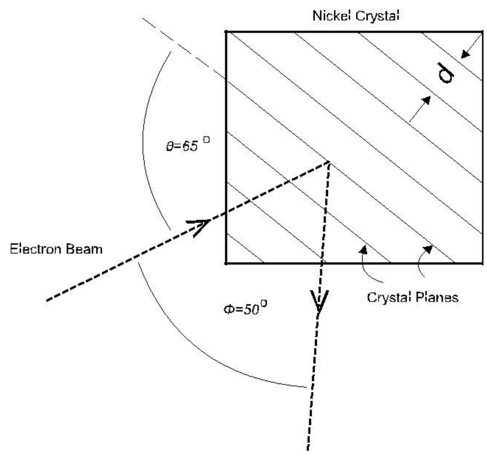
Initially, when accelerating potential was 40 V a smooth curve was obtained. When potential was increased to 44 V ionization current started to increase and reaches maximum for the accelerating potential of 54 V. The scattering angle corresponding to the accelerating Potential 54 V when Ionization current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

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

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

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



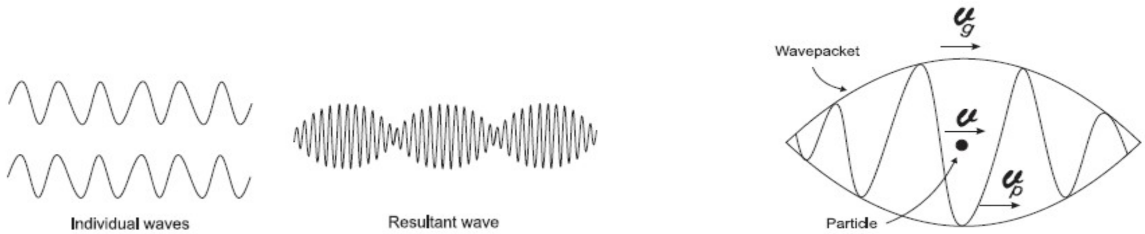
2 sin d n θ λ = where d = Interplanar spacing for the crystal, θ = glancing angle made by incident beam with the crystal plane, n=order and λ is wavelength of the wave. Thus, when bump in the curve is maximum, θ = 65^0 (see fig of crystal), n=1 and for nickel crystal, d = 0.91 .A^0

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

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

Group velocity and Phase velocity

If we have a wave packet, i.e., a wave which is confined to a small volume, it would suppose that the particle is within the region of the wave packet. The position of the particle would then be approximately determined by the position of the wave packet. Thus, it turns out that in quantum mechanics, a particle will be described as a wave packet.



Amplitude variation after Superposition-Wave packet

Each of the component wave propagates with a definite velocity called ***Wave velocity*** or ***Phase velocity*** v_p. The expression for phase velocity is given by, $v_p = \frac{\omega}{k}$.

When a wave packet or group consists of a number of component waves each travelling with slightly different velocity, the wave packet (group) travels with a velocity different from the velocities of component waves of the group. This velocity of the group is called ***Group velocity*** v_g. *The group velocity of a wave is the velocity with which the overall shape of the wave's amplitudes — known as the modulation or envelope of the wave propagates through space.*

Relation between Group velocity and Particle velocity:

We know that, $v_g = \left(\frac{d\omega}{dk}\right)$

But, $\omega = 2\pi\nu = 2\pi\frac{E}{h}$

$$\therefore\ d\omega = \left(\frac{2\pi}{h}\right)dE \tag{16}$$

Also, we have, $k = \frac{2\pi}{\lambda} = 2\pi\left(\frac{p}{h}\right)$ $\qquad \because \lambda = \frac{h}{p}$

$$\therefore dk = \left(\frac{2\pi}{h}\right)dp \tag{17}$$

Dividing Eq.(16) by Eq. (17), we get,

$$\frac{d\omega}{dk} = \frac{dE}{dp} \qquad (18)$$

We also know that, $E = \frac{p^2}{2m}$, where, p is the momentum of the particle.

$$\therefore \frac{dE}{dp} = \frac{2p}{2m} = \frac{p}{m}$$

Using the above equation in Eq. (28), we have,

$$\frac{d\omega}{dk} = \frac{p}{m}$$

But, $p = mv_{particle}$, where v_{particle} is the velocity of the particle.

$$\therefore \frac{d\omega}{dk} = \frac{mv_{particle}}{m} = v_{particle} \qquad (19)$$

From Eq. (25) and Eq. (29), it is clear that,

$$v_{group} = \frac{d\omega}{dk} = v_{particle} \quad \Rightarrow \quad v_{group} = v_{particle} \qquad (20)$$

Thus, the de Broglie wave group associated with an atomic particle travels with a velocity equal to the velocity of the particle itself in a non-dispersive medium.

Again, taking the phase velocity, $v_p = \frac{\omega}{k}$

But, $\omega = 2\pi\left(\frac{E}{h}\right)$ and $k = 2\pi\left(\frac{p}{h}\right)$

$$\therefore v_p = \frac{E}{p} = \frac{mc^2}{mv_{particle}} = \frac{c^2}{v}$$

But from Eq. (20), $v_{group} = v_{particle}$

Hence, $\boxed{v_p v_g = c^2}$

This is the relation connecting group velocity, phase velocity and the velocity of light.

Relation between Group velocity and Phase velocity:

The phase velocity is given by $$v_p = \frac{\omega}{k}$$

$$\Rightarrow \quad \omega = k\, v_p$$

The group velocity is given as,

$$v_g = \frac{d\omega}{dk} = \frac{d}{dk}\left(k v_p\right)$$

$$v_g = v_p + k\frac{dv_p}{dk} \tag{21}$$

But $k = \frac{2\pi}{\lambda}$. $\Rightarrow \quad dk = -\frac{2\pi}{\lambda^2}d\lambda$ and $\frac{k}{dk} = -\frac{\lambda}{d\lambda}$

Using the above relation in Eq. (21), we get,

$$\boxed{v_g = v_p - \lambda\frac{dv_p}{d\lambda}} \tag{22}$$

This is the relation between group velocity and the phase velocity.

Characteristics of matter waves:

- Waves associated with moving particles are called matter waves. The wavelength ‘λ’ of a de-Broglie wave associated with particle of mass ‘m’ moving with velocity 'v' is $\lambda = h/(mv)$
- Matter waves are not **electromagnetic waves** because the de Broglie wavelength is independent of charge of the moving particle and they move with variable velocity.
- The velocity of matter waves (v_P) is not constant. The wavelength is inversely proportional to the velocity of the moving particle ie. $v_{phase} = \frac{c^2}{v_{particle}}$ Which indicates that phase velocity is always greater that c, indicating matter waves are not **physical waves.**
- The phase velocity of matter waves may differ depending upon the mass and velocity of the particle.
- The amplitude of the matter waves at a particular region and time depends on the probability of finding the particle at the same region and time. Therefore matter waves are called as **probability waves.**

- For a particle at rest the wavelength associated with it becomes infinite. This shows that only moving particle produces the matter waves.

Quantum Mechanics

Heisenberg's Uncertainty Principle:

According to classical mechanics a particle occupies a definite place in space and possesses a definite momentum. If the position and momentum of a particle is known at any instant of time, it is possible to calculate its position and momentum at any later instant of time. The path of the particle could be traced. This concept breaks down in quantum mechanics leading to Heisenberg's Uncertainty Principle according to which "It is impossible to measure simultaneously both the position and momentum of a particle accurately. If we make an effort to measure very accurately the position of a particle, it leads to large uncertainty in the measurement of momentum and vice versa.

If Δx and ΔP_x are the uncertainties in the measurement of position and momentum of the particle then the uncertainty can be written as

$$\Delta x \,.\, \Delta P_x \geq (h/4\pi)$$

In any simultaneous determination of the position and momentum of the particle, the product of the corresponding uncertainties inherently present in the measurement is equal to or greater than $h/4\pi$.

Similarly 1) $\Delta E.\Delta t \geq h/4\pi$ 2) $\Delta L.\Delta\theta \geq h/4\pi$

<u>Application of Uncertainty Principle: Non-existence of electrons in the atomic nucleus:</u>

According to the theory of relativity, the energy E of a particle is: $E = mc^2 = \dfrac{m_o c^2}{\sqrt{1-\left(v^2/c^2\right)}}$

Where 'm_o' is the rest mass of the particle and 'm' is the mass when its velocity is 'v'.

$$\text{i.e. } E^2 = \frac{m_o^2 c^4}{1-\left(v^2/c^2\right)} = \frac{m_o^2 c^6}{c^2 - v^2} \qquad \rightarrow (1)$$

If 'p' is the momentum of the particle:

$$\text{i.e. } p = mv = \frac{m_o \text{v}}{\sqrt{1-\left(\text{v}^2/c^2\right)}}$$

$$p^2 = \frac{m_o^2 \text{v}^2 c^2}{c^2 - \text{v}^2}$$

Multiply by c^2

$$p^2c^2 = \frac{m_o^2 \text{v}^2 c^4}{c^2 - \text{v}^2} \qquad \rightarrow (2)$$

Subtracting (2) by (1) we have

$$E^2 - p^2c^2 = \frac{m_o^2 c^4 (c^2 - \text{v}^2)}{c^2 - \text{v}^2}$$

$$E^2 = p^2c^2 + m_o^2c^4 \qquad \rightarrow (3)$$

Heisenberg's uncertainty principle states that

$$\Delta x \,.\, \Delta p_x \geq \frac{h}{4\pi} \rightarrow (4)$$

The radius of the nucleus is of the order 5 x 10^{-15}m. If an electron is to exist inside the nucleus, the uncertainty in its position Δx must not exceed 5 x 10^{-15}m.

$$\text{i.e.} \quad \Delta x \leq 5 \text{ x } 10^{-15}\text{m}$$

The minimum uncertainty in the momentum

$$(\Delta p_x)_{\min} \geq \frac{h}{4\pi \ (\Delta x)_{\max}} \geq \frac{6.63\times10^{-34}}{4\pi\times10^{-14}} \geq 1.1 \times 10^{-20} \text{ kg. m/s} \qquad \rightarrow (5)$$

By considering minimum uncertainty in the momentum of the electron

$$\text{i.e.,} \quad (\Delta P_x)_{\min} \geq 1.1 \times 10^{-20} \text{ kg.m/s} = \text{p} \qquad \rightarrow (6)$$

Consider eqn (3)

$$E^2 = p^2c^2 + m_o^2c^4 = c^2(p^2+m_o^2c^2)$$

Where m_o= 9.11 × 10^{-31} kg

If the electron exists in the nucleus its energy must be

$$E^2 \geq (3 \times 10^8)^2[(1.1 \times 10^{-20})^2 + (9.11 \times 10^{-31})^2(3 \times 10^8)^2]$$

The second term in the bracket can be neglected as it is smaller by more than the 3 orders of the magnitude compared to first term.

Taking square roots on both sides and simplifying

$$E \geq 3.3 \times 10^{-12}\ J \ \geq\ 20.6\ MeV$$

If an electron exists in the nucleus its energy must be greater than or equal to 20.6 MeV. It is experimentally measured that the beta particles ejected from the nucleus during beta decay have energies of about 3 to 4 MeV. This shows that electrons cannot exist in the nucleus.

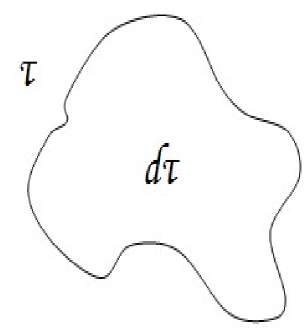
Wave Function:

A wave is constituted by the periodic oscillation of a particular physical quantity. For eg, in case of water waves, the quantity that varies is the height of the water surface, in sound waves it is the pressure variation and in case of electromagnetic waves it is the variation of electric and magnetic fields.

A physical situation in quantum mechanics is represented by a function called wave function. It is denoted by 'ψ'. It accounts for the wave like properties of particles.

Physical significance of wave function:

Probability density: If ψ is the wave function associated with a particle, then $|\psi|^2$ is the probability of finding a particle in unit volume. If 'τ' is the volume in which the particle is present but where it is exactly present is not known. Then the probability of finding a particle in certain elemental volume $d\tau$ is given by $|\psi|^2 d\tau$. Thus $|\psi|^2$ is called probability density. The probability of finding an event is real and positive quantity. In the case of complex wave functions, the probability density is $|\psi|^2 = \psi * \psi$ where ψ^* is complex conjugate of ψ.



Normalization:

The probability of finding a particle having wave function 'ψ' in a volume '$d\tau$' is '$|\psi|^2 d\tau$'. If it is certain that the particle is present in finite volume 'τ', then

$$\int_0^\tau |\psi|^2 d\tau = 1$$

If we are not certain that the particle is present in finite volume, then

$$\int_{-\infty}^{\infty} |\psi|^2 d\tau = 1$$

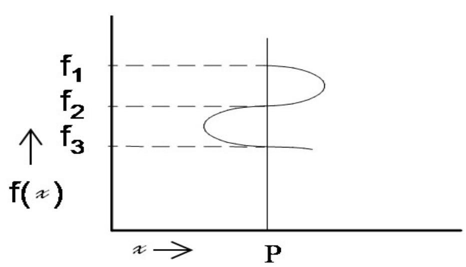
In some cases $\int |\psi|^2 d\tau \neq 1$ and involves constant.

The process of integrating the square of the wave function within a suitable limits and equating it to unity the value of the constant involved in the wave function is estimated. The constant value is substituted in the wave function. This process is called as normalization. The wave function with constant value included is called as the normalized wave function and the value of constant is called normalization factor.

<u>Properties of the wave function:</u>

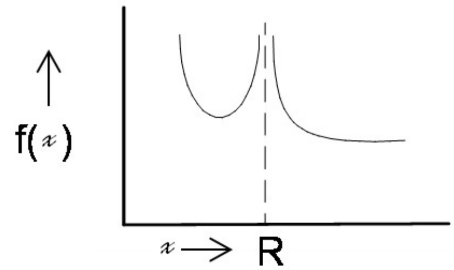
A system or state of the particle is defined by its energy, momentum, position etc. If the wave function 'ψ' of the system is known, the system can be defined. The wave function 'ψ' of the system changes with its state. To find 'ψ' Schrodinger equation has to be solved. As it is a second order differential equation, there are several solutions. All the solutions may not be correct. We have to select those wave functions which are suitable to the system. The acceptable wave function has to possess the following properties:

1) **<u>'ψ' is single valued everywhere</u>**: Consider the function f(x) which varies with position as represented in the graph. The function f(x) has three values f_1, f_2 and f_3 at x = p. Since $f_1 \neq f_2 \neq f_3$ it is to state that if f(x) were to be the wave function. The probability of finding the particle has three different values at the same location which is not true. Thus the wave function is not acceptable.

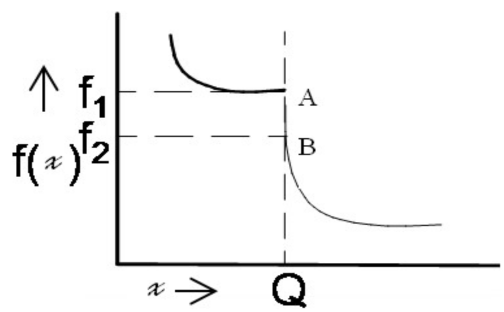


2) **<u>'ψ' is finite everywhere</u>**: Consider the function f(x) which varies with position as represented in the graph. The function f(x) is not finite at x=R but f(x)=∞. Thus it indicates

large probability of finding the particle at a location. It violates uncertainty principle. Thus the wave function is not acceptable.



3) **<u>'ψ' and its first derivatives with respect to its variables are continuous everywhere</u>:** Consider the function f(x) which varies with position as represented in the graph. The function f(x) is truncated at x=Q between the points A & B, the state of the system is not defined. To obtain the wave function associated with the system, we have to solve Schrodinger wave equation. Since it is a second order differential wave equation, the wave function and its first derivative must be continuous at x=Q. As it is a discontinuous wave function, the wave function is not acceptable.



4) For bound states 'ψ' must vanish at potential boundary and outside. If 'ψ*' is a complex function, then ψ* ψ must also vanish at potential boundary and outside.

The wave function which satisfies the above 4 properties are called *Eigen functions*.

<u>Eigen functions:</u>

Eigen functions are those wave functions in Quantum mechanics which possesses the properties:

1. They are single valued.
2. Finite everywhere and
3. The wave functions and their first derivatives with respect to their variables are continuous.

Eigen values:

According to the Schrodinger equation there is more number of solutions. The wave functions are related to energy E. The values of energy E_n for which Schrodinger equation solved are called Eigen values.

Time independent Schrodinger's wave equation

Consider a particle of mass 'm' moving with velocity 'v'. The de-Broglie wavelength 'λ' is

$$\lambda = \frac{h}{m\text{v}} = \frac{h}{p} \rightarrow (1)$$

Where 'mv' is the momentum of the particle.

The wave eqn is

$$\psi = A\, e^{i(kx - \omega t)} \rightarrow (2)$$

Where 'A' is a constant and 'ω' is the angular frequency of the wave.

Differentiating equation (2) with respect to 't' twice

$$\frac{d^2\psi}{dt^2} = -A\omega^2 e^{i(kx-\omega t)} = -\omega^2\psi \rightarrow (3)$$

The equation of a travelling wave is

$$\frac{d^2y}{dx^2} = \frac{1}{\text{v}^2}\frac{d^2y}{dt^2}$$

Where 'y' is the displacement and 'v' is the velocity.

Similarly for the de-Broglie wave associated with the particle

$$\frac{d^2\psi}{dx^2} = \frac{1}{\text{v}^2}\frac{d^2\psi}{dt^2} \rightarrow (4)$$

where 'ψ' is the displacement at time 't'.

From eqns (3) & (4)

$$\frac{d^2\psi}{dx^2} = -\frac{\omega^2}{\text{v}^2}\psi$$

But ω = 2πυ and v =υ λ where 'υ' is the frequency and 'λ' is the wavelength.

$$\frac{d^2\psi}{dx^2} = -\frac{4\pi^2}{\lambda^2}\psi \text{ or } \frac{1}{\lambda^2} = -\frac{1}{4\pi^2\psi}\frac{d^2\psi}{dx^2} \rightarrow (5)$$

$$K.E = \frac{1}{2}m\mathrm{v}^2 = \frac{m^2\mathrm{v}^2}{2m} = \frac{p^2}{2m} \rightarrow (6)$$

$$= \frac{h^2}{2m\lambda^2} \rightarrow (7)$$

Using eqn (5)

$$K.E = \frac{h^2}{2m}\left(-\frac{1}{4\pi^2\psi}\right)\frac{d^2\psi}{dx^2} = -\frac{h^2}{8\pi^2 m\psi}\frac{d^2\psi}{dx^2} \rightarrow (8)$$

Total Energy E = K.E + P.E

$$E = -\frac{h^2}{8\pi^2 m\psi}\frac{d^2\psi}{dx^2} + V$$

$$E - V = -\frac{h^2}{8\pi^2 m\psi}\frac{d^2\psi}{dx^2}$$

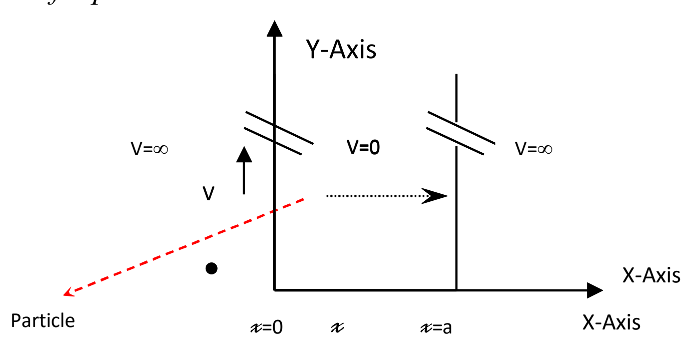
$$\frac{d^2\psi}{dx^2} = -\frac{8\pi^2 m}{h^2}(E-V)\psi$$

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

which is the time independent Schrodinger's wave equation.

Application of Schrodinger wave equation:

Energy Eigen values of a particle in one dimensional, infinite potential well (potential well of infinite depth) or of a particle in a box.



Consider a particle of a mass 'm' free to move in one dimension along positive x-direction between x=0 to x=a. The potential energy outside this region is infinite and within the region is zero. The particle is in bound state. Such a configuration of potential in space is called infinite potential well. It is also called particle in a box. The Schrödinger equation outside the well is

$$\frac{d^2\psi}{dx^2}+\frac{8\pi^2 m}{h^2}(E-\infty)\psi=0 \rightarrow (1) \qquad \because V=\infty$$

For outside, the equation holds good if $\psi = 0$ & $|\psi|^2 = 0$. That is particle cannot be found outside the well and also at the walls

The Schrodinger's equation inside the well is:

$$\frac{d^2\psi}{dx^2}+\frac{8\pi^2 m}{h^2}E\psi=0 \rightarrow (2) \qquad \because V=0$$

$$-\frac{h^2}{8\pi^2 m}\frac{d^2\psi}{dx^2}=E\psi \rightarrow (3)$$

This is in the form $\hat{H}\psi = E\psi$

This is an Eigen-value equation.

Let $\frac{8\pi^2 m}{h^2}E=k^2$ in eqn (2)

$$\frac{d^2\psi}{dx^2}+k^2\psi=0$$

The solution of this equation is:

$$\psi = C\cos kx + D\sin kx \rightarrow (4)$$

at $x = 0 \rightarrow \psi = 0$

$$0 = C\cos 0 + D\sin 0$$

$\therefore$ C = 0

Also $x = a \rightarrow \psi = 0$

$$0 = C\cos ka + D\sin ka$$

But C = 0

$\therefore$ D sin ka = 0 $\longrightarrow$ (5)

D≠0 (because the wave concept vanishes)

i.e. ka = $n\pi$ where n = 0, 1, 2, 3, 4… (Quantum number)

$$k = \frac{n\pi}{a} \rightarrow (6)$$

Using this in eqn (4)

$$\psi_n = D \sin \frac{n\pi}{a} x \rightarrow (7)$$

which gives permitted wave functions.

To find out the value of D, normalization of the wave function is to be done.

$$\text{i.e. } \int_0^a \left|\psi_n^2\right| dx = 1 \rightarrow (8)$$

using the values of ψ_n from eqn (7)

$$\int_0^a D^2 \sin^2 \frac{n\pi}{a} x dx = 1$$

$$D^2 \int_0^a \left[\frac{1-\cos(2n\pi/a)x}{2}\right] dx = 1 \qquad \because \sin^2\theta = \left(\frac{1-\cos 2\theta}{2}\right)$$

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

$$\frac{D^2}{2}\left[x - \frac{a}{2n\pi}\sin\frac{2n\pi}{a}x\right]_0^a = 1$$

$$\frac{D^2}{2}\left[a-0\right] = 1$$

$$\frac{D^2}{2} a = 1$$

$$D = \sqrt{\frac{2}{a}}$$

Hence the normalized wave functions of a particle in one dimensional infinite potential well is:

$$\psi_n = \sqrt{\frac{2}{a}} \sin\frac{n\pi}{a} x \rightarrow (9)$$

Energy Eigen values:

From Eq. 6 & 2

$$\frac{8\pi^2 m}{h^2}E = k^2 = \frac{n^2\pi^2}{a^2}$$

Implies $$E = \frac{n^2h^2}{8ma^2}$$

***Wave functions, probability densities and energy levels for particle in an infinite potential well*:**

Let us consider the most probable location of the particle in the well and its energies for first three cases.

Case I → n=1

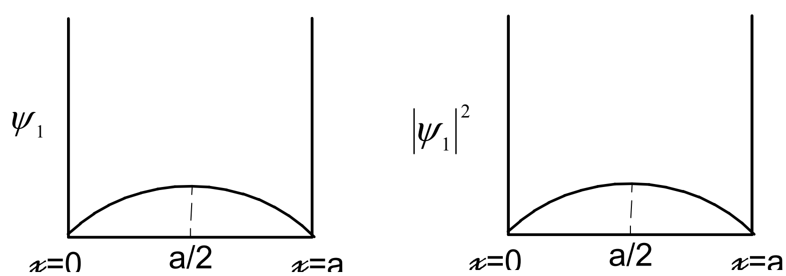
It is the ground state and the particle is normally present in this state.

The Eigen function is

$\psi_1 = \sqrt{\frac{2}{a}}\sin\frac{\pi}{a}x$ ∵ from eqn (7)

$\psi_1 = 0$ for $x = 0$ and $x = a$

But ψ_1 is maximum when $x = a/2$.



The plots of ψ_1 versus x and $|\psi_1|^2$ verses x are shown in the above figure.

$|\psi_1|^2 = 0$ for $x = 0$ and $x = a$ and it is maximum for $x = a/2$. i.e. in ground state the particle cannot be found at the walls, but the probability of finding it is maximum in the middle.

The energy of the particle at the ground state is

$$E_1 = \frac{h^2}{8ma^2} = E_0$$

Case II → n=2

In the first excited state the Eigen function of this state is

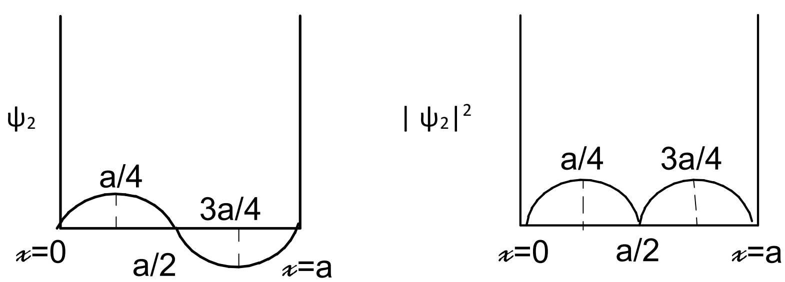
$$\psi_2 = \sqrt{\frac{2}{a}} \sin \frac{2\pi}{a} x$$

$\psi_2 = 0$ for the values $x = 0, a/2, a$.

Also ψ_2 is maximum for the values $x = a/4$ and $3a/4$.

These are represented in the graphs.

$|\psi_2|^2 = 0$ at $x = 0, a/2, a$, i.e. particle cannot be found either at the walls or at the centre. $|\psi_2|^2 =$maximum $for\ x = \frac{a}{4}, x = \frac{3a}{4}$



The energy of the particle in the first excited state is $E_2 = 4E_0$.

Case III → n=3

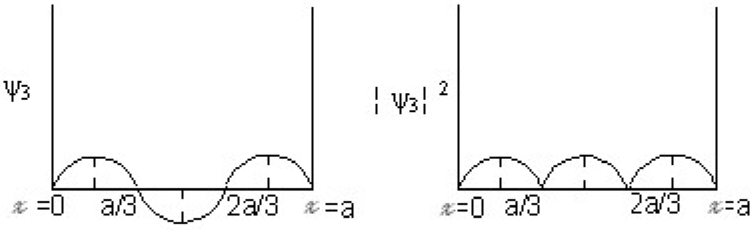
In the second excited state,

$$\psi_3 = \sqrt{\frac{2}{a}} \sin \frac{3\pi}{a} x$$

$\psi_3 = 0$, for $x = 0, a/3, 2a/3$ and a.

ψ_3 is maximum for $x = a/6, a/2, 5a/6$.

These are represented in the graphs.



$|\psi_3|^2 = 0$ for $x = 0$, a/3, 2a/3 and a. $|\psi_3|^2 = \text{maximum} \; for \; x = \frac{a}{6}, x = \frac{a}{2}, x = \frac{5a}{6}$

The energy of the particle in the second excited state is $E_3 = 9 E_0$.

Energy Eigen values of a free particle:

A free particle is one which has zero potential. It is not under the influence of any force or field i.e. V = 0.

The Schrodinger equation is:

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} E\psi = 0$$

or $$-\frac{h^2}{8\pi^2 m}\frac{d^2\psi}{dx^2} = E\psi$$

This equation holds good for free particle in free space in which V = 0.

With the knowledge of the particle in a box or a particle in an infinite potential well V = 0 holds good over a finite width 'a' and outside V = ∞. By taking the width to be infinite i.e. a = ∞, the case is extended to free particle in space. The energy Eigen values for a particle in an infinite potential well is

$$E = \frac{n^2 h^2}{8ma^2}$$

Where n =1, 2, 3, …

$$n = \frac{2a}{h}\sqrt{2mE}$$

Here when 'E' is constant, 'n' depends on 'a' as a→∞ n→∞. It means that free particle can have any energy. That is the energy Eigen values or possible energy values are infinite in number. It follows that energy values are continuous. It means that there is no discreteness or quantization of energy. Thus a free particle is a *'Classical entity'*.