BMS INSTITUTE OF TECHNOLOGY & MANAGEMENT
(Autonomous Under VTU)

Module-2 (Autonomous-CSE stream)

Quantum mechanics

<u>Dual nature of matter (de-Broglie Hypothesis)</u>

Light exhibits the phenomenon of interference, diffraction, photoelectric effect and Compton Effect. The phenomenon of interference, diffraction can only be explained with the concept that light travels in the form of waves. The phenomenon of photoelectric effect and Compton Effect can only be explained with the concept of *Quantum theory of light.* It means to say that light possess particle nature. Hence it is concluded that light exhibits dual nature namely wave nature as well as particle nature.

<u>de-Broglie's Wavelength:</u>

A particle of mass 'm' moving with velocity 'c' possess energy given by

$E = mc^2 \quad \rightarrow$ **(**Einstein's Equation) (1)

According to Planck's quantum theory the energy of quantum of frequency 'υ' is

$E = h\upsilon \quad \rightarrow (2)$

From (1) & (2)

$mc^2 = h\upsilon = hc/\lambda \qquad \text{since } \upsilon = c/\lambda$

$\lambda = hc/mc^2 = h/mc$

$\lambda = h/mv \qquad \text{since } \; v \approx c$

<u>Relation between de-Broglie wavelength and kinetic energy</u>

Consider an electron in an electric potential V, the energy acquired is given by

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

Where 'm' is the mass, 'v' is the velocity and 'p' is the momentum of the particle. 'e' is charge of an electron.

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

The expression for de-Broglie wavelength is given by

$$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{h}{\sqrt{2meV}} = \frac{h}{\sqrt{2mE}}$$

de-Broglie Wavelength of a charged particles like electron / proton etc.,:-

An electron accelerated with potential difference ‘V’ has energy ‘eV’. If ‘m’ is the mass and ‘v’ is the velocity of the electron.

Then $eV = 1/2(mv^2) \quad \rightarrow (1)$

If ‘p’ is the momentum of the electron, then p=mv

Squaring on both sides, we have

$p^2 = m^2v^2$

$mv^2 = p^2/m$

Using in equation (1) we have

$eV = p^2/(2m)$ or $p = \sqrt{(2meV)}$

According to de-Broglie $\lambda = h/p$

Therefore $\lambda = \left[\frac{h}{\sqrt{2meV}}\right] = \frac{1}{\sqrt{V}}\left[\frac{h}{\sqrt{2me}}\right]$

For electron

$$\lambda = \frac{1}{\sqrt{V}}\left[\frac{6.626\times10^{-34}}{\sqrt{2\times9.11\times10^{-31}\times1.602\times10^{-19}}}\right]$$

$$= \frac{1.226\times10^{-9}}{\sqrt{V}}\,\mathrm{m}$$

$$\boxed{\lambda = \frac{1.226}{\sqrt{V}}\,\mathrm{nm}}$$

de-Broglie Wavelength of a neutral particle like neutron:-

$$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{h}{\sqrt{2meV}} = \frac{h}{\sqrt{2mE}}$$

Where E for neutral particles can be treated as similar to kinetic theory of gas molecules given by $E = \frac{3}{2} K_B T$; where K_B is Boltzmann constant = 1.38×10^{-23} J/K and T is the temperature. By substituting this in the above equation then

$$\lambda = \frac{h}{\sqrt{3mk_B T}}$$

Characteristics of matter waves:

1. 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

   $\lambda = h/(mv)$

2. Matter waves are not electromagnetic waves because the de Broglie wavelength is independent of charge of the moving particle.
3. The velocity of matter waves (v_P) is not constant. The wavelength is inversely proportional to the velocity of the moving particle.
4. Lighter the particle, longer will be the wavelength of the matter waves, velocity being constant.
5. For a particle at rest the wavelength associated with it becomes infinite. This shows that only moving particle produces the matter waves.

Phase velocity – definition & expression

Phase velocity: The velocity with which individual wave travels in group of waves is called phase velocity.

In a travelling wave, the velocity with which the phase is propagated is called phase velocity (V_{ph})

The phase velocity is equal to $\gamma\lambda$

Ie $V_{ph} = \gamma\lambda$ -------------------(1)

But we know that angular velocity or angular frequency

$\omega = 2\pi\gamma$ or $\gamma = \frac{\omega}{2\pi}$ --------------------(2)

Similarly, propagation constant or wave number is given by

$k = \frac{2\pi}{\lambda}$ or $\lambda = \frac{2\pi}{k}$ -------------(3)

By substituting equations 2 and 3 in 1, we get

$$V_{ph} = \frac{\omega}{2\pi} \times \frac{2\pi}{k}$$

$V_{ph} = \frac{\omega}{k}$, hence, phase velocity is the ratio of angular frequency and propagation constant.

Group velocity definition and expression

The velocity with which resultant envelop of the group of waves travel is called group velocity. Schrodinger postulated that a moving particle (e^-, etc) is equivalent to a wave packet rather than a single wave. Hence, group velocity is equal to particle velocity.

The group velocity is denoted as $V_g = \frac{d\omega}{dk}$.

Relation between group velocity and phase velocity

Group velocity is given by

$V_g = \frac{d\omega}{dk}$ ----------------(1)

Phase velocity is given by

$V_{ph} = \frac{\omega}{k}$ ------------------(2)

Where ω – angular velocity or angular frequency

k – Propagation constant or wave number or wave vector.

From equation 2 , $\omega = V_{ph} k$ ----------- (3)

Substituting equation 3 in 1, we get

$V_g = \frac{d\omega}{dk} = \frac{d(V_{ph}k)}{dk} = V_{ph} + k\frac{dV_{ph}}{dk}$ ------------(4)

But $k = \frac{2\pi}{\lambda}$ -------------------------------(5)

By differentiating with respect to λ

$dk = -\frac{2\pi}{\lambda^2} d\lambda$ ----------------(6)

Substituting equation 5 and 6 in 4

$V_g = V_{ph} - \lambda\frac{dV_{ph}}{d\lambda}$. This equation gives the relation between phase velocity and group velocity.

Relation between group velocity and particle velocity:

The equation between group velocity and phase velocity is

$V_g = \frac{d\omega}{dk}$ --------------------------------(1)

But angular frequency $\omega = 2\pi\gamma$ -----------------(2)

From plank's theory of radiation $E = h\gamma \Rightarrow \gamma = \frac{E}{h}$ -------------------(3)

Substituting γ from equation 3 in equation 2, we get

$\omega = 2\pi\frac{E}{h}$

On differentiating, $d\omega = \frac{2\pi}{h} dE$ ------------------(4)

We know the equation of propagation constant

$k = \frac{2\pi}{\lambda}$ ------------(5)

$\lambda = \frac{h}{p}$ ---------(6)

Substituting λ value from equation 6 in equation 5

$k = 2\pi \frac{p}{h}$

On differentiating

$dk = \frac{2\pi}{h} dp$ ------------------------(7)

Dividing equation 4 by 7

$\frac{d\omega}{dk} = \frac{dE}{dp}$ -----------(8)

We know that , E=$\frac{1}{2} m v_p^2$ or $E = \frac{p^2}{2m}$

Where 'p' is momentum of the particle. By differentiating, we get,

$dE = \frac{2p}{2m} dp$ (or) $dE = \frac{p}{m} dp$ (or) $\frac{dE}{dp} = \frac{p}{m}$

But p = $mv_{particle}$

Hence $\frac{dE}{dp} = \frac{mv_p}{m} = v_p$ -----------------(9)

Comparing equations 1, 8 and 9

$V_g = v_p$, ie group velocity is equal to particle velocity.

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/4π.

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

Physical Significance of Heisenberg's principle:

1) it is not possible to determine accurately and simultaneously the values of position and momentum of a particle at any time. If we want to determine the position of an electron very accurately then this can be done at the expense of accuracy in determining its momentum and vice versa.
2) The uncertainty leads to probability function that is probability of finding the particle at a certain position or probable value for the momentum of the particle.
3) Uncertainty principle make us to understand that matter and light / radiation are two sides of a coin
4) Uncertainty principle helps us to sub atomic particle.

Application of Uncertainty Principle:

Impossibility of existence of electrons in the atomic nucleus:

According to the theory of relativity, the energy E of a particle is:

$$E = mc^2 = \frac{m_o c^2}{\sqrt{1-\left(v^2/c^2\right)}}$$

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

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

If 'p' is the momentum of the particle:

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

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

Multiply by c^2

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

Subtracting (2) by (1) we have

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

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

Heisenberg's uncertainty principle states that

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

The diameter of the nucleus is of the order 10^{-14}m. If an electron is to exist inside the nucleus, the uncertainty in its position Δx must not exceed 10^{-14}m.

i.e. $\Delta x \leq 10^{-14}$m

The minimum uncertainty in the momentum

$$(\Delta P_x)_{\min} \geq \frac{h}{4\pi\ (\Delta x)_{\max}} \geq \frac{6.63\times10^{-34}}{4\pi\times10^{-14}} \geq 0.5 \times 10^{-20}\ \text{kg. m/s} \rightarrow (5)$$

By considering minimum uncertainty in the momentum of the electron

i.e., $(\Delta P_x)_{\min} \geq 0.5 \times 10^{-20}$ kg.m/s = p $\rightarrow$ (6)

Consider eqn (3)

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

Where $m_o = 9.11 \times 10^{-31}$ kg

If the electron exists in the nucleus its energy must be

$$E^2 \geq (3 \times 10^8)^2[(0.5 \times 10^{-20})^2 + (9.11 \times 10^{-31})^2(3 \times 10^8)^2]$$

i.e. $E^2 \geq (3 \times 10^8)^2[0.25 \times 10^{-40} + 7.4629 \times 10^{-44}]$

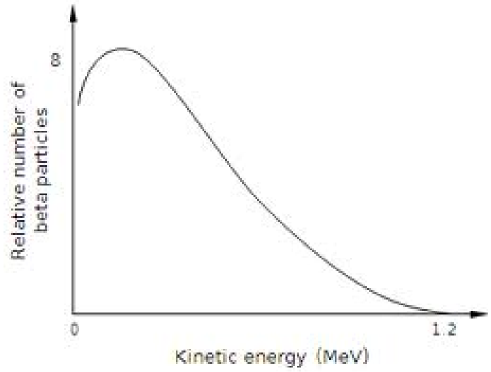
Neglecting the second term as it is smaller by more than the 3 orders of the magnitude compared to first term.

Taking square roots on both sides and simplifying

$$E \geq 1.5 \times 10^{-12}\ \text{J} \geq \frac{1.5\times10^{-12}}{1.6\times10^{-19}}\ \text{ev} \geq 9.4\ \text{Mev}$$

If an electron exists in the nucleus its energy must be greater than or equal to 9.4Mev. 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.

[**Beta decay:** In beta decay process, from the nucleus of an atom, when neutrons are converting into protons in releasing an electron (beta particle) and an antineutrino. When proton is converted into a neutron in releasing a positron (beta particle) and a neutrino. In both the processes energy sharing is statistical in nature. When beta particles carry maximum energy neutrino's carries minimum energy and vice-versa. In all other processes energy sharing is in between maximum and minimum energies. The maximum energy carried by the beta particle is called as the end point energy (E_{max}).



Principle of Complementarity:

Complementarity is an interesting concept that was introduced by Neils Bohr in the year 1928. Now let us explain the principle of complementarity or Bohr's complementarity principle. We know that the consequence of the uncertainty principle is both the wave and particle nature of the matter cannot be measured simultaneously. In other words, we cannot precisely describe the dual nature of light. Now suppose that an experiment is constructed in such a way that it is designed to measure the particle nature of the matter. This implies that, during this experiment, errors of measurement of both position and the time coordinates must be zero or absent, this in turns explains that the momentum, energy and the wave nature of the matter are completely unknown. Similarly, if an experiment is designed for measuring the wave nature of the particle, then the errors in the measurement of the energy and the momentum will be zero, whereas the position and the time coordinates of the matter will be completely unknown.

From the above explanation, we can conclude that, when the particle nature of the matter is measured or displayed, the wave nature of the matter is necessarily suppressed and vice versa. The inability to observe the wave nature and the particle nature of the matter simultaneously is known as the complementarity principle. It was first explained by Niels Bohr in the year 1928 and hence it is familiarly known as the Bohr's Complementarity principle.

Wave Function:

Wave function is a mathematical tool used in quantum mechanics to describe any physical system. A physical situation in quantum mechanics is represented by a function called wave function. It denotes the function of momentum, time, position, and spin. It is denoted by 'ψ'. It accounts for the wave like properties of particles. Wave function is obtained by solving Schrodinger equation. To solve Schrodinger equation, it is required to know

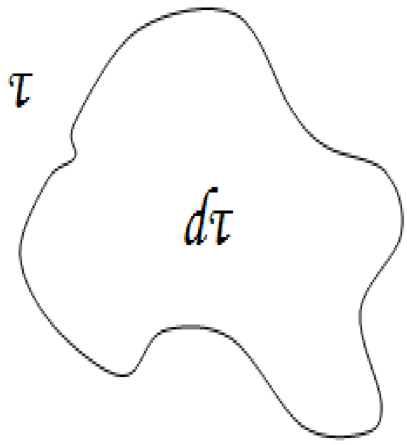
1) Potential energy of the particle

2) Initial conditions and

3) Boundary conditions.

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

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

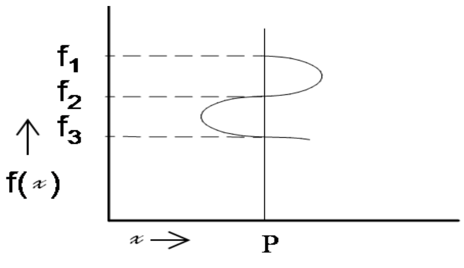
In some cases $\int |\psi|^2 d\tau \neq 1$ and involves constant.

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 wavefunction. 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.

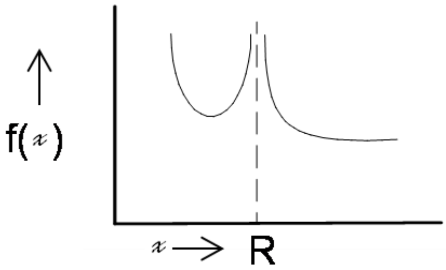
Properties of the wave function:

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:

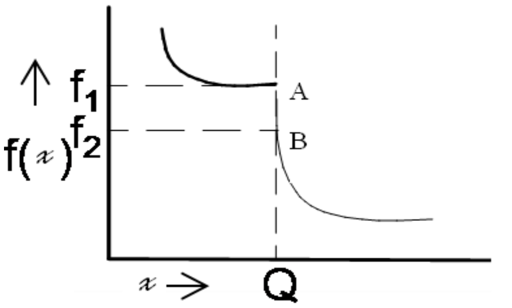
1) 'ψ' is single valued everywhere: Consider the function f(x) which varies with position as represented in the graph. The function f(x) has three values f_1, f_2 and f_3 at x = p. Since $f_1 \neq f_2 \neq f_3$ it is to state that if f(x) were to be the wave function. The probability of finding the particle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



2) 'ψ' is finite everywhere: 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 and Eigen values:-</u>

Eigen value equations are those equations in which on the operating of a function by an operator, we get function back only multiplied by a constant value. The function is called Eigen function and the constant value is called Eigen value. Eigen functions 'ψ' 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.

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.

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.

Operator (quantity)	Classical definition	Quantum operator
Position	R	r
Linear momentum	P	$-i\hbar\frac{\partial}{\partial x}$ or $-i\hbar\nabla$
Angular momentum	r ×p	$-i\hbar(r\times\nabla)$
Kinetic energy	$\frac{p^2}{2m}$	$-\frac{\hbar^2}{2m}\nabla^2$
Potential energy	V	V
Total energy (time dependent)	E	$i\hbar\frac{\partial}{\partial t}$
Hamiltonian (time independent)	$H=\frac{p^2}{2m}+V$	$-\frac{\hbar^2}{2m}\nabla^2+V$

There are two types of Schrodinger equations:

1) ***The time dependent Schrodinger equation:*** It takes care of both the position and time variations of the wave function. It involves imaginary quantity *i*.

The equation is: $$-\frac{h^2}{8\pi^2 m}\frac{d^2\psi}{dx^2}+V\psi=-\frac{ih}{2\pi}\frac{d\psi}{dt}$$

2) ***The time independent Schrodinger equation*****:** It takes care of only position variation of the wave function.

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

Time independent Schrodinger wave equation

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

$$\lambda=\frac{h}{m\mathrm{v}}=\frac{h}{P}\longrightarrow(1)$$

Where 'mv' is the momentum of the particle.

The wave eqn is

$$\psi=Ae^{i(kx-\omega t)}\longrightarrow(2)$$

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

Differentiating equation (2) with respect to ‘t’ twice

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

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.

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

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

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

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

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

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

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

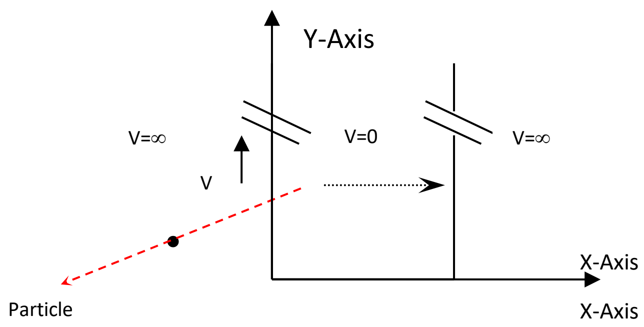
$$\boxed{\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0}$$

Which is the time independent Schrodinger wave equation.

Application of Schrodinger wave equation:

PARTICLE IN ONE-DIMENSIONAL POTENTIAL BOX:-

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

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

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

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

$D \neq 0$ (because the wave concept vanishes)

i.e. $ka = n\pi$ where $n = 0, 1, 2, 3, 4\ldots$ (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.

i.e. $\int_0^a |\psi_n^2| dx = 1 \longrightarrow (8)$

using the values of ψ_n from eqn (7)

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

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

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

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

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

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

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

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

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

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

Alternative Method (Operator method) (Additional Information)

Energy Eigen values are obtained by operating the wave function 'ψ' by the energy operator (Hamiltonian operator).

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

Inside the well 0 < x < a, V=0

$$\hat{H} = -\frac{h^2}{8\pi^2 m}\frac{d^2}{dx^2} \rightarrow (10)$$

The energy Eigen value eqn is

$$\hat{H}\psi = E\psi \rightarrow (11)$$

From equation (10) and (11)

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

i.e. $-\frac{h^2}{8\pi^2 m}\frac{d^2\psi_n}{dx^2} = E\psi_n \rightarrow (12)$

It is the Eigen value equation.

Differentiating eqn (9)

$$\frac{d\psi_n}{dx} = \sqrt{\frac{2}{a}}\frac{n\pi}{a}\cos\frac{n\pi}{a}x$$

Differentiating again

$$\frac{d^2\psi_n}{dx^2} = -\sqrt{\frac{2}{a}}\left(\frac{n\pi}{a}\right)^2 \sin\frac{n\pi}{a}x$$

$$\frac{d^2\psi_n}{dx^2} = -\left(\frac{n\pi}{a}\right)^2 \psi_n$$

Using this eqn. in (12)

$$\frac{h^2}{8\pi^2 m}\left(\frac{n\pi}{a}\right)^2 \psi_n = E\psi_n$$

$$E = \frac{n^2 h^2}{8ma^2} \rightarrow (13)$$

It gives the energy Eigen values of the particle in an infinite potential well.

n = 0 is not acceptable inside the well because $\psi_n = 0$. It means that the electron is not present inside the well which is not true. Thus the lowest energy value for *n* = 1 is called zero-point energy value or ground state energy.

i.e. $E_{zero\text{-}point} = \frac{h^2}{8ma^2}$

The states for which n >1 are called exited states.

$E_1, E_2, E_3 \ldots.$

<u>Wave functions, probability densities and energy levels for particle in an infinite potential well</u>:

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

<u>Case I → n=1</u>

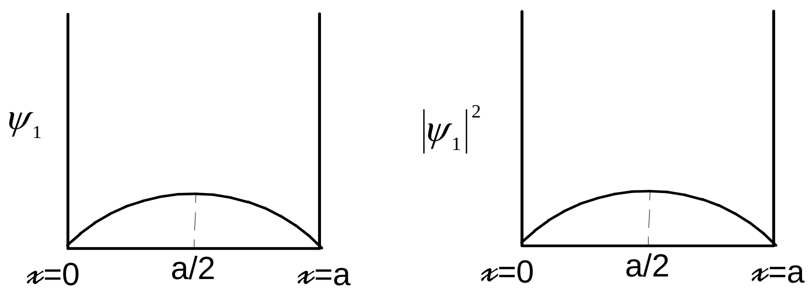
It is the ground state and the particle is normally present in this state.

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

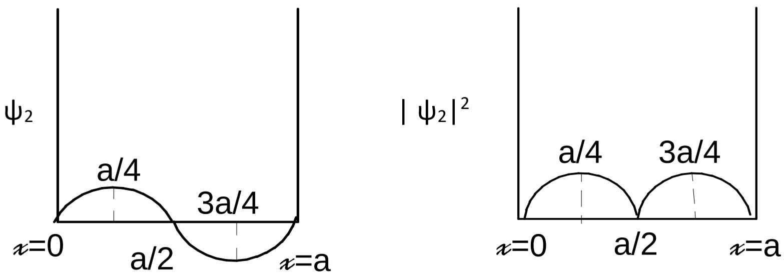
$$\psi_2 = \sqrt{\frac{2}{a}} Sin \frac{2\pi}{a} x$$

$\psi_2 = 0$ 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

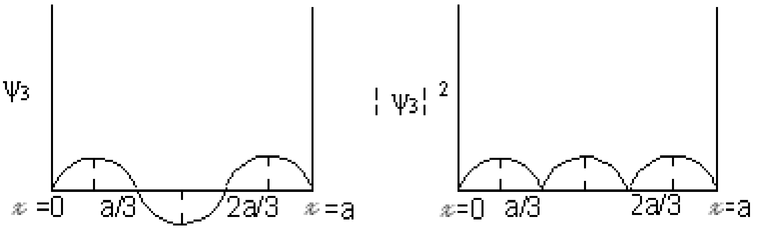
In the second excited state,

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

$\psi_3 = 0$, 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. $|\psi_3|^2$ =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'*.

Numericals:-

1. Calculate the number of photons emitted in 3 hrs. by a 60 watt sodium lamp. Given λ=589.3nm.

2. Light of wavelength $4047A^0$ falls on a photoelectric cell with a sodium cathode. It is found that the photoelectric current ceases when a retarding potential of 1.02 volt is applied. Calculate the work function of the sodium cathode.

3. The most rapidly moving valence electron in metallic sodium at absolute zero temperature has a kinetic energy 3eV. Show that the de Broglie wavelength is $7A^0$.

4. Calculate the momentum of an electron possessing the de Broglie wavelength 6.62×10^{-11}m.

5. Find the phase and group velocities of an electron whose de-Broglie wavelength is 0.12nm.

6. Find the kinetic energy and group velocity of an electron with de-Broglie wavelength of 0.2nm (Jan 2011)

7. Calculate the wavelength of a 1kg object whose velocity is 1m/s and compare it with the wavelength of an electron accelerated by 100 volt ($\lambda_0=6.62 \times 10^{-34}$ m, $\lambda_e = 1.2 \times 10^{-10}$m and $\lambda_e = 1.8 \times 10^{23}\ \lambda_0$)

8. Calculate the de-Broglie wavelength associated with 400 gm cricket ball with a speed of 90Km/hr. (VTU August 2006)

9. Compare the energy of a photon with that of an electron when both are associated with wave length of 0.2nm. (VTU Feb 2006, August 2003, IAS- 1987)

10. Compare the energy of a photon with that of a neutron when both are associated with wave length of 0.1nm. Given the mass of neutron is 1.678×10^{-27}kg. (Jan 2009)

11. Calculate the wavelength associated with electrons whose speed is 0.01 of the speed of light. (VTU August 2004)

12. The velocity of an electron of a Hydrogen atom in the ground state is 2.19 x 10^6m/s. Calculate the wavelength of the de Broglie waves associated with its motion.

13. Compute the de Broglie wavelength for a neutron moving with one tenth part of the velocity of light (June-July 2011)

14. Estimate the potential difference through which a proton is needed to be accelerated so that its de Broglie wavelength becomes equal to $1A^0$, given that its mass is 1.673 x 10^{-27}kg.

15. Calculate the de Broglie wavelength associated with an electron with a kinetic energy of 2000eV. (VTU March 2006)

16. Evaluate de Broglie wavelength of Helium nucleus that is accelerated through 500V.

17. A particle of mass 0.511 MeV/c^2 has kinetic energy 100eV. Find its de-Broglie wavelength, where c is the velocity of light. (VTU Jan 2007, IAS 1978)

18. Compare the momentum, the total energy, and the kinetic energy of an electron with a de-Broglie wavelength of $1A^0$, with that of a photon with same wavelength.

19. Calculate the de Broglie wavelength of a proton whose kinetic energy is equal to the rest energy of the electron. Mass of proton is 1836 times of electron.

20. A fast moving neutron is found to have an associated de Broglie wavelength of 2 x 10^{-12}m. Find its kinetic energy, the phase and group velocities of the de Broglie waves ignoring the relativistic change in mass. Mass of neutron= 1.675 x 10^{-27}kg.

21. Two copper nanowires are insulated by a copper oxide nano-layer that provides a 10.0-eV potential barrier. Estimate the tunneling probability between the nanowires by 7.00-eV electrons through a 5.00-nm thick oxide layer. What if the thickness of the layer were reduced to just 1.00 nm? What if the energy of electrons were increased to 9.00 eV?

22. A proton with kinetic energy 1.00 eV is incident on a square potential barrier with height 10.00 eV. If the proton is to have the same

transmission probability as an electron of the same energy, what must the width of the barrier be relative to the barrier width encountered by an electron?

23. If an electron has a de Broglie wavelength of 3 nm, find its kinetic energy and group velocity, given that it has rest mass energy of 511 kev.(Dec 2010)

24. A Particle of mass 0.65 MeV/c^2 has kinetic energy 80eV. Find the de Broglie wavelength, group velocity and phase velocity of the de Broglie wave. (VTU Model Question Paper, Jan 2008, July 2008)

25. An electron has a wavelength of 1.66 x 10^{-10}m. Find the kinetic energy, phase velocity and group velocity of the de Broglie wave. (VTU August 1999)

26. Calculate the wavelength associated with an electron having kinetic energy 100eV. (VTU July 2002)

27. Calculate the wavelength associated with an electron raised through a potential difference of 2 kV. (VTU Feb 2002)

28. Find the energy of an electron moving in one dimension in an infinitely high potential box of width 1.0 A^0. (Ans:- 37.694 n^2 eV)
29. A spectral line of wavelength 546.1nm has a width 10-5nm. Estimate the minimum time spent by electrons in the excited state during transitions. (July 2007,Dec 2010)
30. An electron is bound in a one dimensional potential box which has a width 2.5 x 10-10m. Assuming the height of the box to be infinite, calculate the two lowest permitted energy values of the electron. (Ans:- 6.04eV and 24.16eV)
31. Calculate the lowest energy of a neutron confined to the nucleus, where nucleus is considered a box with a size of 10-14m. (Ans:- 6.15Mev)
32. Estimate the time spent by an atom in the excited state during the excitation and de-excitation processes, when a spectral line of wavelength 546 nm and width 10-14 is emitted (Jan 2011).
33. A particle is in motion along a line between x=0 and x=a with zero potential energy. At points for which x<0 and x>a, the potential energy is infinite. The wave function for the particle in the nth state is given by

$$\Psi_n = D \sin\left(\frac{n\pi}{a}x\right)$$

Find the expression for the normalized wave function.

34. Show that $\phi(x) = e^{ikx}$ is acceptable eigen-function, where k is some finite constant. For a region -a≤ x ≤a; normalize the given eigen-function.
35. A particle is moving in one dimensional potential well of infinite height and of width 25A0. Calculate the probability of finding the particle in an interval of 5 A0 at a distances of a/2, a/3 and a , where a is the width of the well assuming that the particle is in its least state of energy.(Ans:- P1=0.3871, P2= 0.2937 and P3=0.0086)
36. A quantum particle confined to one-dimensional box of width 'a' is in its first excited state. What is the probability of finding the particle over an interval of (a/2) marked symmetrically at the centre of the box (Jan 2011).

<u>Questions:-</u>

1. State and explain the Heisenberg uncertainty principle. Using this principle, show that the electrons cannot reside in an atomic nucleus. (Jan 2007, Jan 2011)
2. State the exact statement of Heisenberg uncertainty principle. Name three pairs of physical variables for which this law holds true.
3. Derive time-independent Schrödinger wave equation. What is the physical significance of state function 'ψ' used in this equation? What conditions must it fulfill?
4. What is a wave function? Explain the properties of wave function? (July 2007,June 2011)
5. Write down the Schrödinger equation for a particle in one-dimensional box. Obtain the eigen functions and eigen values for this particle.
6. A particle is moving freely within one-dimensional potential box. Find out the eigen functions of the particle and show that it has discrete eigen values.
7. Find the expression for the energy state of a particle in one-dimensional box.
8. What do you mean by an operator? Write the operators associated with energy and momentum.
9. Set up time-independent one-dimensional Schrödinger equation.
10. What is normalization of a wave function? What are the physical significance and properties of wave function?
11. What are eigen values and eigen functions? Discuss the nature of eigen values and eigen functions.
12. Give the Max Born's interpretation of wave function and explain the normalization conditions.

13. Solve the Schrödinger wave equation for the allowed energy values in the case of particle in a box. (June 2011)
14. Using Schrödinger wave equation for a particle in one-dimensional well of infinite height, discuss about energy eigen values.
15. Describe zero-point energy.
16. Assuming the time independent Schrödinger wave equation, discuss the solution for a particle in one-dimensional potential well of infinite height. Hence obtain the normalized wave function (Jan 2008)
17. What is the physical interpretation of wave function? How a free particle wave function signifies a particle in space and momentum?
18. Solve the Schrödinger wave equation for the one-dimensional potential well defined by

$$V(x) = \infty \qquad \text{for } x < 0 \text{ and } x > a$$

$$V(x) = 0 \qquad \text{for } 0 \leq x \leq a$$

19. Find the Eigen value and Eigen functions for an electron in one dimensional potential well of infinite height (July 2007,Jan 2011)
20. Discuss the wave functions, probability densities and energy levels for a particle in a box. (Jan 2007)