BASICS OF QUANTUM MECHANICS T.Y.B.Sc

***Q.1.* Give a brief account of the historical developments of quantum mechanics.**

Ans. The historical developments of quantum mechanics can be accounted by taking into consideration the various theories put forward to explain the structure of atom.

In **1800**,***John Dalton*** proposed his atomic theory that matter is composed of hard, indivisible tiny particles called atoms. With the further developments in the study of atomic structure, in **1896**, ***Sir J.J. Thomson*** discovered electron and proposed the existence of proton. In **1900**, ***Max Planck*** proposed his quanum theory that radiation is emmited by matter in the form of packets of energy called photons or quantas. This can be considered as the **first stage** in the development of quantum mechanics. In **1905**, ***Albert Einstein*** used Plank's ideas and explained the photoelectric effect sucessfully.He applied Plank's hypothesis to explain the low temperature specific heat of solids.Einstein concept of photoelectric effect was not explained successfully by the then known classical mechanics which explained the motion of objects(size greater than 10^{-10} m) in terms of Newton's Laws of motion and electromagnetic theory of light.

In **1911**,***Lord Rutherford's*** experiment of scattering of alpha particles established the stability of atom which did not fit in the framework of classical mechanics. In **1913**, ***Sir Neils Bohr*** applied quantum theory to explain the structure of atom.He proposed that an electron in an atom revolves in concentric circular orbits called **stationary orbits.**The energy of the electron in an orbit is quantised and its angular momentum is an integral multiple of **nh/2π**.Thus Bohrs theory forms the foundation of old quantum theory which could succesfully explained the structue of hydrogen atom. However it failed to explain the structure of those atoms posessing more than one electron.

In **1923**, ***A.H.Compton*** confirmed Plank's view that light radiation consist of particles called photons .This can be considered as the begining of the idea that light has **dual** character ie particle as well as wave.

The **second stage** of quantum mechanics started in **1925** with the introduction of matrix mechanics by Werner Heisenberg.He laid down the concept that **" it is impossible to determine simultaneously and precisely the momentum and the position of a microscopic particle."**

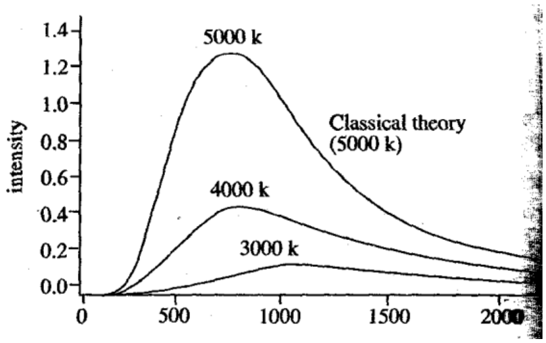
If Δx is the uncertainty regarding the position and Δp is the uncertainty about the momentum then according to Heisenberg's uncertainty principle: $\mathbf{\Delta x . \Delta p = h / 2\pi}$ **where h is the Planck's constant.**

In **1924**,***Louis de Broglie*** suggested that wave-particle dual nature of radiation could also be applied to the matter. De-Broglie showed that a particle of mass m moving with velocity v is associated with a wavelength λ given by $\lambda = \frac{h}{m.v} \rightarrow (1)$

where h is the Planck's constant. This equation is called de Broglie equation which is a fundamental equation of wave-particle duality.The waves exhibiting dual nature were called **matter waves**.***Davisson, Germer and Thomson*** in **1927** confirmed the existance of matter waves.***Schrodinger*** in **1926** further extended De Broglies ideas and derived an equation for matter wave.This equation provided a systematic and quantitative approach replacing the old quantum theory.Thus two different ways of working with quantum mechanics was evolved. The first was proposed by **Heisenberg** and is called **matrix mechanics** while the second based on **Schrodinger** wave equation and is known as **wave mechanics**.

Q.2) Explain the limitations of classical mechanics with reference to black body radiation.

Ans: A black body is a blackened surface which absorbs and emit radiations perfectly. It is found that the intensity of radiation emitted per unit surface area of a black body depends only on temperature and independent of nature of the solid. A typical spectrum of the black body is as shown below:



From the above spectrum, following conclusions can be drawn:

1) At any temperature T, energy density increases with the frequency of light emitted, reaches maximum and then falls to zero.

2) With the increase in temperature, the peak shifts to a higher frequency indicating high intensity of radiation emitted.

The above two observations are contrary to classical mechanics because it assumes that intensity of light emitted and hence its energy will increase at infinite rate with increase in temperature.

Q.3) Explain photoelectric effect. What are the limitations of classical mechanics on this effect? How they are overcome by quantum theory?

Ans: When a beam of light of certain frequency is incident on the surface of the metal like alkali metals, electrons are emitted from the metal surface. This phenomenon is called photoelectric effect. The classical mechanics interpreted this effect in the following manner:

i) The emission of electrons from the metal surface is independent of the incident wavelength of light and depends on the intensity of incident radiation.

ii) The increase in intensity of incident radiation increases the number of electron emission and not its energy.

However, Einstein explains this effect on quantum basis which assumes that the incident radiation is composed of particles called photons. Light of any wavelength or frequency will not emit electrons but a certain frequency called threshold frequency is necessary to observed the effect. The conclusions on the basis of quantum theory are as follows:

i) Every metal surface has a threshold frequency which depends on the nature of the metal surface below which the effect is not observed.

ii) The photons of the incident beam transfer energy to electrons on the metal surface which drags them out from the metal surface. The energy of the electrons emitted depends on the frequency of radiation and not on intensity.

Q.4) Describe the Compton effect. How is it justified by quantum theory?

Ans: When a beam of high energy radiation like X ray is incident on the surface of the metal, it was observed that the scattered beam from the metal surface has a wavelength greater than the wavelength of incident radiation.This effect was observed by Compton and is called Compton effect.

The classical electromagnetic theory interpreted the effect in the following way:

i) The wavelength of the incident and the scattered beam should be same.

ii) The scattering should show a symmetrical distribution with respect to intensiry.

However, Compton could explain the effect by considering the radiations to be made up of particles called photons.The high energy photons of the incident beam collide with the loosely bound electron of the atom and transfer their energy and momentum to them, which then recoil.The new photons thus produce have less energy and momentum and therefore the scattered beam has longer wavelength.Thus according to quantum theory, the change in wavelength produced due to scattering is independent of the incident wavelength.

Q.5) Distinguish between matter waves and electromagnetic waves.

Ans

Sr.No.	Matter waves	Electromagnetic waves
1	These waves are associated with every material particle in motion	These are waves emitted or absorbed by atoms or molecules under consideration
2	Their speed is much less than electromagnetic waves	Their speed is much higher than matter waves
3	They do not travel in vacuum	They travel in vacuum
4	Their wavelength is much smaller as compared to electromagnetic wave	Their wavelength is spread over the entire range which gives rise to electromagnetic spectrum.

Q.6) Describe the theory of wave motion as applicable to quantum mechanics.

Ans. Quantum mechanics is a science which deals with the motion of micro particles such as an electron, proton etc. The theories laid down by Heisenberg and De Broglie in quantum mechanics suggest than an electron is not only a particle but also exhibit the properties of a wave. Thus an electron is characterized by wavelength, frequency, wave number etc.The wave properties exhibited by an electron suggest that there must be a wave equation and wave function for it similar to that observed for waves of light, sound and strings. The source of this wave motion is of vibratory type, the simplest of which is the simple harmonic motion. It is a periodic motion, which assumes a definite value after a definite period of time.

Consider a stretched string whose one end is fixed while at the other end, a weight is attached supported by a spring. The weight moves freely up and down in a vertical direction. This vertical displacement from its mean position is called amplitude of vibration which is a function of position as well as time and is denoted by $\psi_{(x,t)}$.

Diagram

When the weight is pulled down by a distance **'l'** and released, it executes a simple harmonic motion of certain time **T** and moves in a vertical direction.The wave moves a dicstance of one wavelength in time T.The velocity 'v' of the wave is given by

$$\mathbf{v = \lambda/T} \quad \text{where } \lambda \text{ is the } \textbf{wavelength} \text{ of the wave.}$$

But frequency $\nu = 1/T$

$$\therefore \quad v = \nu . \lambda$$

The moving wave is a progressive wave along the X axis whose amplitude $\psi_{(x,t)}$. is a product of two functions

$$\text{i.e} \quad \psi_{(x,t)} = \psi_{(x)} . \Phi_{(t)}$$

where $\psi_{(x)}$ is a function of **x** only and $\Phi_{(t)}$ is a function of t only. $\psi_{(x)}$ is independent of t and $\Phi_{(t)}$ is independent of x. Such types of wave motions are described quantitatively by the second order differential equation as follows

$$\frac{\partial^2 \psi(x,t)}{\partial x^2} = \frac{1}{c^2} . \frac{\partial^2 \psi(x,t}{\partial t^2} \quad \rightarrow (1)$$

In the above equation, Ψ is the amplitude function and it measures the variation of displacement along the y-axis at a particular distance x along the X-axis,c is the velocity of the wave and t is the time.

The above equation is linear and gives several solutions on solving. The general solution of the differential equation is given by

$$\psi = A \sin 2\pi(x/\lambda - \nu T) \qquad \text{-----------------(2)}$$

where λ is the wavelength of the wave, A is the amplitude of the wave and ν is the frequency of the wave.

The equation **(2)** represents a plane wave moving from left to right. A similar wave moving from right to left can be represented by

$$\psi = A \sin 2\pi \ (x/\lambda + \nu t) \qquad \text{-----------------------(3)}$$

When two waves one represented by equation (2) and the other by equation (3) move in opposite directions with the same speed, then the resultant amplitude will be given by

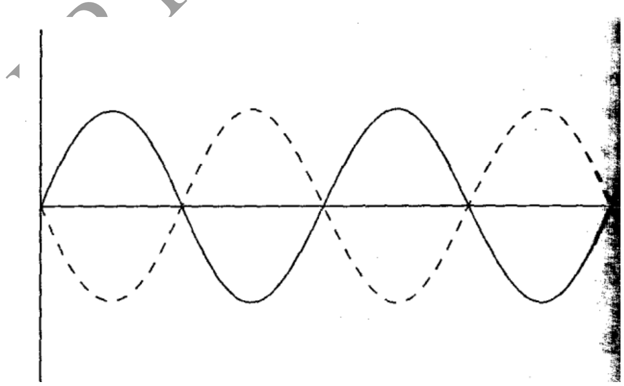
$$\psi = A \sin 2\pi \ (x/\lambda - \nu t) + A \sin 2\pi \ (x/\lambda + \nu t)$$

$$\psi = 2A \sin 2\pi \frac{x}{\lambda} . \cos 2\pi\nu t \qquad \text{---------------------} \qquad (4)$$

The equation (4) correspond to wave which does not move either forward or backward is known as standing or stationary wave.

Definition of stationary wave: The waves whose amplitude is a function of position only and independent of time are called stationary waves.

Diagram of simple harmonic wave:



Q.7)What is an harmonic oscillator?Give the comparitive study of classical and quantum mechanical operator?

Ans. When a particle oscillates about its mean position along a straight line under the action of a force which **i)** is directed towards the mean position and **ii)** is proportional to the displacement at any instant from this position, the motion of the particle is said to be simple harmonic and the oscillating particle is called a simple harmonic oscillator. For such an oscillator, wave mechanics shows that the vibrational energy is related to the fundamental vibration frequency ν_0 by the relation

$$E_\nu = (\nu + ½)h\nu_0$$

where ν is vibrational quantum number, which may take the values ν = 0,1,2,etc.The above equation reveals that such an oscillator retains in its lowest vibrational level ν=0 with energy

$$E_0 = ½ h\nu_0$$

Comparison of classical oscillator and wave- mechanical oscillator

Classical oscillator	**Wave mechanical operator**
1.Energy changes continuosly and it	1.Energy can have discrete values only.
can have any value.	
2. The maximum displacement is fixed	2.Particle can exist anywhere. There is a finite probability of finding the
called amplitude which depends upon	particle in classically forbidden region.
Energy	Here the potential energy is greater
	than total energy.
3. Minimum energy is zero and particle	3.Minimum energy is ½ hω called zero t
is at rest in this state.	Energy.Here particle cannot be at rest
	because of uncertainity principle

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Q.8)Obtain the following solutions for Ψ(x) and φ(t) using the method of seperation of two variables.

Ans.The equation for propogation of a wave along X axis will represent an equation showing the variation of the amplitude of the wave with respect to both position and time. Let **Ψ** (x,t) represent the amplitude of the propagating wave ie displacement along Y axis. By method of separation, **Ψ** (x,t) can be separated into two separate equations. The function Ψ (x,t) is a product of two functions i.e. $\psi(x,t) = \Psi(x).\ \varphi(t)$ ------- **(1)**

where $\Psi(x)$ is a function of x only and $\varphi(t)$ is a function of t only. The general differential equation for the function Ψ (x,t) is given by

$$\frac{\partial^2 \psi(x,t)}{\partial x^2} = \frac{1}{c^2} \cdot \frac{\partial^2 Q(x,t)}{\partial t^2} \quad \text{------- (2)}$$

As $\Psi(x)$ and $\varphi(t)$ are independent of each other, we have

$$\frac{\partial \Psi(x,t)}{\partial x} = \varphi(t).\ \frac{d\,[\Psi(x)]}{dx}$$

and

$$\frac{\partial \Psi}{\partial t} = \Psi(x)\ .\ \frac{d}{dt}\varphi(t)$$

$$\frac{\partial^2 \psi(x,t)}{\partial x^2} = \varphi(t).\frac{d^2\Psi(x)}{dx^2} \quad \text{---------(3)}$$

Similarly, $$\frac{\partial^2 \Psi(x,t)}{\partial t^2} = \Psi(x).\frac{d^2}{dt^2}\varphi(t) \quad \text{----------(4)}$$

Substituting the terms of equation of **3 and 4** in equation 1, we get

$$\varphi(t)\ .\frac{d^2\Psi(x)}{dx^2} = \frac{\Psi(x).}{c^2}\ \frac{d^2}{dt^2}\varphi(t)$$

On rearrangement, we get

$$\frac{c^2}{\Psi(x)} \cdot \frac{d^2\Psi(x)}{dx^2} = \frac{1}{\varphi(t)}\ \frac{d^2\varphi(t)}{dt^2}$$

As the above equation contains two variables and two functions on L.H.S. and R.H.S seperately, each side must be equal to a constant term.

$$\therefore\ \frac{c^2}{\Psi(x)} \cdot \frac{d^2\Psi(x)}{dx^2} = \frac{1}{\varphi(t)}\ \frac{d^2\varphi(t)}{dt^2} = -k^2 \quad \text{-----------(4)}$$

This gives rise to two separate equations

$$\frac{c^2}{\Psi(x)} \cdot \frac{d^2\Psi(x)}{dx^2} = -k^2$$

$$\frac{1}{\varphi(t)} \cdot \frac{d^2\varphi(t)}{dt^2} = -k^2$$

$$\frac{d^2\Psi(x)}{dx^2} + \frac{k^2\,\Psi(x)}{c^2} = 0 \text{ and}$$

$$\frac{d^2\varphi(t)}{dt^2} + k^2\,\varphi(t) = 0$$

The above equations are second order differential equations which have several solutions as follows:

$$\Psi(x) = A \sin(k/c\,.x)$$

$$\Psi(x) = A \cos(k/c\,.x)$$

$$\Psi(x) = A \operatorname{Sin}(k/c\,.x) + B.\cos(k/c\,.x)$$

$$\Psi(x) = A\,e^{\pm ikx}$$

Similar equations can be written for $\varphi(t)$

Among the various solutions obtained, the general solution accepted is

$$\Psi(x) = A \operatorname{Sin}(k/c\,.x) + B.\cos(k/c\,.x) \qquad \text{-------------}(5)$$

Similarly for $\varphi(t)$, the general solution accepted is

$$\varphi(t) = C \sin(kt) + B \cos(kt) \qquad \text{---------------}(6)$$

The above equations are periodic in nature.

Therefore, the time period of the wave **$T = 2\pi/k$**

Hence frequency $\nu = 1/T = k/2\pi$

$$\therefore \lambda = 2\pi c/k$$

Hence $k = 2\pi c/\lambda$

Substituting the values of k in equation 5 and 6, we get

$$\Psi(x) = A \sin(2\pi/\lambda\,.x) + B.\cos(2\pi/\lambda\,.x)$$

and $$\varphi(t) = C \sin(2\pi c/\lambda.t) + B \cos(2\pi c/\lambda.t)$$

Q.9) What is meant by stationary wave? What are the boundary conditions of stationary wave? Sketch the vibrational modes of a clamped string.

Ans. A stationary wave is a wave whose amplitude is a function of position only and independent of time is called a stationary wave. Under such condition, the wave does not propagate hence the name stationary wave.

As electron shows wave like properties, which do not show any variation with time, the electron waves are therefore stationary waves.

For a stationary wave, the following second order differential equation is obeyed

$$\frac{d^2\Psi(x)}{dx^2} + \frac{k^2}{c^2}\Psi(x) = 0 \qquad \text{-----------(1)}$$

The corresponding solution of the equation is given by

$$\Psi(x) = A \sin(2\pi/\lambda\ .x) + B.\cos(2\pi/\lambda\ .x)$$

Consider a stationary wave generated on a stretched string of length L clamped at x=0 and x=L.At these points, the string is not allowed to vibrate.

$$\Psi(x) = 0 \text{ at } x = 0$$

and $$\Psi(x) = L \text{ at } x = L$$

These are known as boundary conditions which can help to find the values of A and B from equation 1

<u>Condition I</u>: $x = 0$ when $\Psi(x) = 0$

$$0 = A \sin(2\pi/\lambda.0) + B\cos(2\pi/\lambda.0)$$

$$= A \sin 0 + B \cos 0$$

As $\sin 0 = 0$ and $\cos 0 = 1$

$$\therefore B = 0$$

Hence $\Psi(x) = A \sin(2\pi/\lambda.x)$

<u>Condition II</u>: $x = L$, $\Psi(x) = 0$

$$\Psi(x) = A \sin(2\pi/\lambda.x)$$

$$0 = A.\sin(2\pi/\lambda.L)$$

Two possibilities arise

Either **$A = 0$** or **$\sin(2\pi/\lambda . L) = 0$**

$A = 0$ is not possible as it will provide **$\Psi(x) = 0$** for all values of x.

Therefore $\sin(2\pi/\lambda . L) = 0$

Hence **$2\pi/\lambda . L = \sin^{-1} 0 = n\pi$** where **n = 0,1,2,3-------**

$$\therefore \lambda = 2L/n$$

Substituting in equation **$\Psi(x) = A \sin(2\pi/\lambda . x)$** we get,

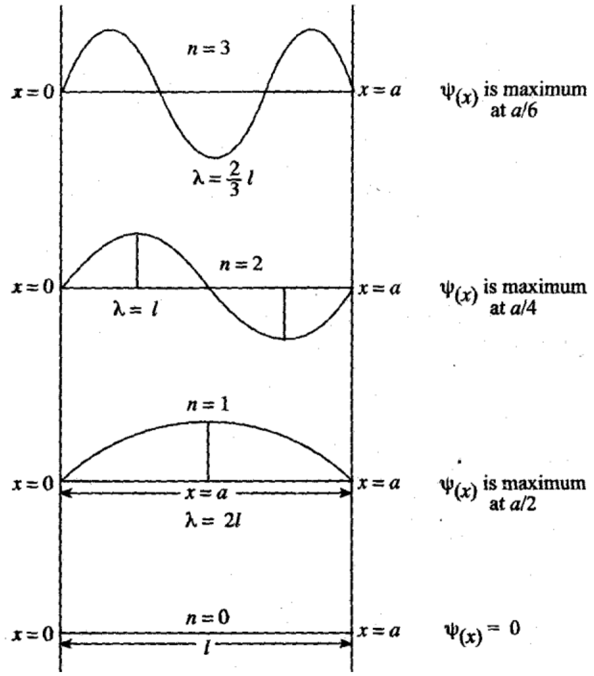
$$\Psi(x) = A \sin(2\pi/ 2L/n . x)$$

$$= A \sin(n\pi/L . x)$$

For different values of n, different modes of vibrations are obtained.

n	No.of nodes	$\Psi(x)$	Position of nodes
1	0	$\Psi(x) = A \sin(\pi/L.x)$	x = 0 and x = L
2	1	$\Psi(x) = A \sin(2\pi/L.x)$	x =0, x = ½, x =L
3	2	$\Psi(x) = A \sin(3\pi/L.x)$	x = 0,x = L/3, x =2L/3 & x = L

Sketch of stationary wave:



Q.10)State the Schrodinger wave equation and explain the physical significance of the wave function.

Ans. According to Erwin Schrondinger, microparticles like electrons, protons etc. have a dual character ie particle as well as wave character.He combined the classical wave time independent wave equation and the de Broglie equation to obtain a time independent wave equation .The equation so obtained was termed as Schrodinger wave equation.

The time independent Schrodinger wave equation is given by the relation:

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

The various terms involved in this equation are as follows:

m = the mass of the particle,

E = Total energy of the particle,

V = Potential energy of the particle,

h = Planck’s constant,

ψ = eigen function or wave function of the particle.

Significance of wave function:

A wave function is a **mathematical function** which may be large in one region,small in others and zero elsewhere. It contains all the information about the location and motion of the particles it describes. If a wavefunction is large at a particular point, then the particle has a high probability of being at that point or if the wave function is zero at a point then the particle will not be found at that point. The more rapidly the wave function changes from place to place, the higher the kinetic energy of the particle it describes.

The wave function Ψ in the Schrodinger equation is a function of position only and independent of time. It may be a complex function or a real one.

i)For the complex function, Ψ takes the form

$$\Psi = a + ib$$

where a and b are real functions of the coordinates and $i = \sqrt{-1}$.

The complex conjugate of Ψ is $\Psi^* = a - ib$

$$\therefore \Psi . \Psi^* = a^2 + b^2$$

Thus the product $\Psi . \Psi^*$ is always real and not a negative quantity.

ii) If Ψ is a real function, then $\Psi = \Psi^*$ hence $\Psi.\Psi^*$ is also equal to Ψ^2.

According to **Max Born**, the square of the wave function (or $\Psi . \Psi^*$**)** at a point is proportional to the probability of finding the particle at that point. Thus Ψ^2 or $\Psi . \Psi^*$ represents the probability density ie it is a measure of the probability of finding the particle(electron) at that point.For a particle to move in three dimensions, the wavefunction depends on the point r with coordinates x, yand z.In such a case, the probability of finding the particle in an infinitesimal volume

dτ =dx.dy.dz at the point **r** is proportional to $\Psi.\Psi^* d\tau$.

The sign of the wave function has no significance but its square is physically important.

The wave function, which satisfies the above conditions, is called well-behaved function.

Q.11)What is well behaved function? Is e^{3x} a well behaved function?

Ans.The Schrodinger equation is a second order differential equation. There are several solutions(wave functions) to this equation but few of them have physical and chemical significance.The wavefunctions which satisfy the following the following conditions are acceptable.

1) Ψ must be finite and single valued for all value of the coordinates.

2) Ψ must be a continuous function of the coordinates.

3) $\int \Psi^2 . d\tau$ must be finite when the integration is carried over the whole space.

The wave function, which satisfies the above conditions, is called well-behaved function.

Such wavefunctions are called Eigen functions of the system.

The function e^{3x} is a well-behaved function, which can be proved as follows;

Let the operator of this function be d^2/dx^2 and let it be multiplied by a constant term k.

Then for e^{3x} to be defined as well behaved function, it must satisfy the following condition

$$\frac{d^2}{dx^2}(e^{3x}) = k.e^{3x}$$

Proof:

$$\frac{d^2}{dx^2}(e^{3x}) = \frac{d}{dx}.\left(\frac{d}{dx}.e^{3x}\right)$$

$$= \frac{d}{dx}(3.e^{3x})$$

$$= 9.e^{3x}$$

Here 9 is the eigen value of the equation and the above equation is called eigen value equation.Thus e^{3x} is a well behaved function.

Q.12)What is an operator? What are the conditions for the operators to be commutative?Why should the operators chosen for the dynamic variables of the system be linear?

Ans. The Schrodinger wave equation explains well the behaviour of one particle system.But for a system with more than one particle, a more general and rigorous mathematical treatement is required in quantum mechanics.For such mathematical study, the concept of operators is required.

An operator is a symbol for a mathematical procedure which changes one function to another.It is denoted by a letter with a cap on it.eg, **Â.**

If **A** and **B** are two operators operating on a function f(x), then the two operators are said to be commutative if

$$\mathbf{A.B\ f(x) = B.A\ f(x)}$$

For example, consider the function f(x) = 2 x .Let A = k and B =d/dx

Â . B f(x) = kx .d/dx(2x) = kx.2 = 2kx

B. A f(x) = 2x.d/dx(kx) = 2x.k = 2kx

In the above case, **A.B f(x)** = **B.A f(x)** therefore **A & B** are said to be commutative.

The operators chosen for the dynamic variables should be linear because the principle of simultaneous measurement of the dynamic properties mainly depends upon two commuting operations. If the operations are not commuting, then it is not possible to determine simultaneously the exact position and momentum of a particle beyond a certain level of precision.

Q.13)Explain the term 'Linear operators'.

Ans.**<u>Linear operator</u>:-** When operating on the sum of two functions, if an operator gives the same result as the sum of the operations on the two functions separately, then the operator is said to be linear.

Suppose f(x) and g(x) are two functions and $\hat{A}$ is an operator, then the operator to be linear the condition is

$$\hat{A}\,(f(x) + g(x)) = \hat{A}\,f(x) + \hat{A}\,g(x)$$

and also

$$\hat{A}\,c\,f(x) = c\,\hat{A}\,f(x)$$

For example, d/dx and integration are linear operators because

$$\frac{d}{dx}[f(x) + g(x)] = \frac{d}{dx} f(x) + \frac{d}{dx} g(x)$$

$$\frac{d}{dx}[a\, f(x)] = a \frac{d}{dx} f(x)$$

Similarly, $\int [f(x) + g(x)]\, dx = \int f(x)\, dx + \int g(x)\, dx$

$$\int c\, f(x)\, dx = c \int f(x)\, dx$$

However taking square is not a linear operator

$$\sqrt{f(x) + g(x)} = \sqrt{f(x)} + \sqrt{g(x)}$$

and $\sqrt{c\, f(x)} = \sqrt{c\, f(x)}$

Q.14) Explain the operator concept. How is addition, multiplication of operators carried out? When do you say that the two operators commute?

Ans. The Schrodinger wave equation explains well the behaviour of one particle system.But for a system with more than one particle, a more general and rigorous mathematical treatement is required in quantum mechanics.For such mathematical study, the concept of operators is required.

An operator is a symbol for a mathematical procedure which changes one function to another.It is denoted by a letter with a cap on it.eg, $\hat{A}$.

For e.g. d/dx is an operator which converts a function into it's first derivative with respect to x. Thus d/dx transforms f (x^n) into f n x^{n-1}. i.e. $\mathbf{\frac{d}{dx} f(x^n) = f\, n\, x^{n-1}}$

In general **(Operator) . (function) = Another function.**

(i) Addition and subtraction of operators is governed by $\mathbf{(\hat{A} + \hat{B})\, f(x) = \hat{A}\, f(X) + \hat{B}\, f(x)}$ and $\mathbf{(\hat{A} - \hat{B})\, f(x) = \hat{A}\, f(x) - \hat{B}\, f(x)}$

For example if $\hat{A} = \log_{10}$ and $\hat{B} = \frac{d}{dx}$ and $f(x) = x^n$ then

$$(\hat{A} + \hat{B})\, f(x) = \hat{A}\, f(x) + \hat{B}\, f(x) = \log_{10} x^n + \frac{d}{dx} x^n = n \log_{10} x + n\, x^{n-1}$$

(ii) When two operators are multiplied, then the two operations are carried out one after another, with order of operation from right to left. Thus A B f(x) involves multiplication

of two operators $\hat{A}$ and $\hat{B}$. **$\hat{A}\hat{B}$ f (x) = $\hat{A}$ [$\hat{B}$ f (x)] = $\hat{A}$ m (x) = n (x)**

It can be seen that function f(x) is first operated by $\hat{B}$ when the function m(x) is obtained.

This on being operated by $\hat{A}$ gives the function n(x).

If A and B are two operators operating on a function f(x), then the two operators are said to be commutative if

$\hat{A}.\hat{B}$ f(x) = $\hat{B}$ $\hat{A}$ f(x)

For example, consider the function f(x) = 2 x.. Let A = k and B =d/dx

$\hat{A}$ $\hat{B}$ f(x) = k x .d/dx(2x) = k x.2 = 2 k x

$\hat{B}$ $\hat{A}$ f(x) = 2x.d/dx(kx) = 2x.k = 2k x

In the above case,AB f(x) = BA f(x) therefore A & B are said to be commutative.

Q.15.If two operators A and B commute, then they have same set of eigen functions.'Explain.

Ans. The operators A and B commute means they satisfy the following condition

$\hat{A}$. $\hat{B}$ f(x) = $\hat{B}$ $\hat{A}$ f(x)

Let the eigen function for the operator A be Ψ .Then the eigen value equation is

$\hat{A}$ Ψ = a. Ψ where a is the eigen value.

Therefore $\hat{A}$. $\hat{B}$ Ψ = $\hat{B}$. A Ψ = B (a. Ψ) =a B Ψ

This shows that B Ψ is an eigen function of the operatorA with an eigen value a.

This is possible when B Ψ is a multiple of Ψ . ie B Ψ = b. Ψ

In other words, Ψ is also an eigen function of B.

Q.16 .What are eigen function and eigen values? Show that the function Ψ = ae$^{x/a}$ is an eigen function of the operator d/dx. What is the eigen value?

Ans.A function **Ψ** is said to be an eigen function of an operator A if it satisfies the following condition

$\hat{A}$. Ψ = a. Ψ

where the constant **a** is called the eigen value equation. The above equation is called eigen value equation.

The eigen function is also termed as state function of the system.The square of the eigen function at a particular region in space will represent the probability of finding the system within that region.

To show that **$\Psi = ae^{x/a}$** is an eigen function of the operator d/dx.

$$\frac{d}{dx}\Psi = \frac{d}{dx}(a.e^{x/a}) = a\frac{d}{dx}(e^{x/a}) = a.\frac{1}{a}e^{x/a} = \frac{1}{a}(a.e^{x/a}) = \frac{1}{a}\Psi$$

Therefore Ψ **i**s an eigen function and its eigen value is **1/a.**

Wave-Particle dualism:- When radiation interacts with matter, it displays particle like properties, in contrast with wave like properties (e.g. interference, diffraction) it exhibits when it propagates. The particle like properties are illustrated by photo electric effect and Compton effect. Thus electromagnetic radiation has a dual nature. In propagation it behaves like a wave and in certain interactions with matter, it behaves like particles.

(1) De-Broglie equation:- In 1924 L. de Broglie suggested that wave particle dual nature of radiation can also be applied to the matter. De-Broglie showed that a particle of mass m moving with velocity V is associated with a wavelength λ given by

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

where h is the Planck's constant. This equation called de Broglie equation is a fundamental equation of wave particle duality.

Equation (1) can e derived as follows:

According to Planck's Quantum theory the energy of photon is given by $E = h\nu$.

Einstein equation for mass energy equivalence gives $E = mc^2$ where c is velocity of light.

$$\therefore h\nu = mc^2 \qquad \rightarrow (2)$$

where m is the mass equivalence of photon.

$$\therefore \frac{hc}{\lambda} = mc^2 \qquad \therefore \lambda = \frac{h}{mc} \qquad \rightarrow (3)$$

De-Broglie suggested that the above equation is applicable to moving particles of matter. Thus for a particle of mass m moving with velocity **v**, the equation **(3)** can be written as

$$\lambda = \frac{h}{m.v} \qquad \rightarrow (4)$$

This equation is the de-Broglie equation.

It can be seen from the de-Broglie equation that for a given velocity, the wavelength is inversely proportional to mass. Consequently, for commonly observable material particles, the wavelengths are so small that it is almost impossible to measure them. The equation (4) can be used to calculate wavelengths of moving sub-atomic particles.

Experimental verification of De Broglie equation:

The De Broglie's hypothesis that an electron also possess a wave like character in addition to its particle behaviour was verified experimentally by Davisson and Germer through electron diffraction grating experiments.In this experiments, a beam of X rays were allowed to pass through a crystal of nickel.A diffraction pattern similar to that exhibited by light waves was observed which proved that electrons possess a wave like character. The expression for wavelength of an electron was obtained as follows:

Consider an electron of charge $\mathbf{e^-}$ accelerated by a potential **V**.The kinetic energy of the electron under this condition is given by **V.e**.

If u is the velocity of the electron, then the kinetic energy will be $1/2mu^2$

Therefore

$$1/2mu^2 = V.e \qquad \text{or}$$

$$u = (2Ve/m)^{1/2}$$

Substituting the value of u in the de Broglie's equation, we get,

$$\lambda = h / m.u$$

$$= \frac{h}{m\,(2V.e/m)^{1/2}}$$

$$= \frac{h}{\sqrt{2.V.e.m}}$$

Substituting **h**= **6.626 X 10^{-34} J.sec**, e=**1.602 x 10^{-19}C**, and **m=9.109 X 10^{-31}kg** we get

$$\lambda = \frac{12.26 \times 10^{-10}}{\sqrt{V}}$$

Where V is the potential in volts.

When V =**100 volts**,

$$\lambda = \frac{12.26 \times 10^{-10}}{\sqrt{100}} = 1.226 \times 10^{-10} = 1.226A^0$$

By varying the potential between **10** and **10,000** volts**, λ** is found to vary between **3.877A^0** to **0.1226A^0** which corresponds to a wavelength of **X ray** region

(2) <u>Heisenberg's Uncertainty Principle</u>:- It states that **" It is impossible to determine simultaneously and precisely the momentum and the position of a microscopic particle."**

If Δx is the uncertainty regarding the position and Δp is the uncertainty about the momentum then according to Heisenberg's uncertainty principle:

$$\Delta x. \Delta p = h / 4\pi$$

But momentum p = mass X velocity = m.v

Therefore $\Delta x. \Delta(m.v) = h / 4\pi$

where h is the Planck's constant.

i.e $\Delta x. m \Delta v = h / 4\pi$

Hence $$\Delta x. \Delta .v = h / 4\pi m \qquad 1$$

The above equation is applicable for a particle of low mass such as an electron which can be shown as follows:

For an electron, mass is **9.109 X 10^{-31}kg**

Substituting the value of m along with the other constant values in equation 1 we get,

$$\Delta x.\ \Delta.v = 6.627 \times 10^{-34} / 4 \times 3.14 \times 9.109 \times 10^{-31} kg$$

$$= 5.792 \times 10^{-5}$$

Thus we find that the product of uncertainty is very high which means certainty is low.

On the other hand, if we apply this equation to a tennis ball of mass 0.01kg, we get

$$\Delta x.\ \Delta.v = 6.627 \times 10^{-34} / 4 \times 3.14 \times 0.01$$

$$= 5.27 \times 10^{-31}$$

Thus the product of uncertainty is very less which means certainty is more.

Thus one can conclude form the above examples that a particle like electron has no definite path because of dual character of the electron i.e particle as well as wave character.

According to uncertainty principle, if the position of a particle such as an electron is precisely known, then there will an uncertainty regarding its momentum. For example, if an electron having an exactly known momentum strikes a fluorescent screen, a flash of light is emitted so that it's position at that instant is exactly known. But as a result of collision of electron with screen, some amount of energy is lost and consequently, the momentum of electron gets changed. Thus in trying to establish the position of electron precisely, an uncertainty is introduces regarding it's momentum. Thus, it is impossible to determine simultaneously and precisely position and momentum of a microscopic particle.

Q.17) Explain the term 'Hamiltonian operator.'

Ans: The total energy of an electron is the sum of its kinetic and potential energy in classical mechanics, the total energy of a particle(eg an electron) is given by the expression

$$\frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + V = E \quad \text{------------}\mathbf{1}$$

The time independent Schrodinger wave equation is given by the relation:

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

On rearranging the above equation we get

$$\frac{-h^2}{8\pi^2 m}\left(\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2} + V\right)\psi = E.\psi \quad \text{---------}2$$

Comparing equation 1 and 2 , we get

$$\frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) = \frac{-h^2}{8\pi^2 m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \quad \text{---------------}3$$

i.e $p_x^2 + p_y^2 + p_z^2 = \frac{-h^2}{4\pi^2 m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$

This indicates that

$$P_x^2 = \frac{-h^2}{4\pi^2 m} \cdot \frac{\partial^2}{\partial x^2}$$

$$P_y^2 = \frac{-h^2}{4\pi^2 m} \cdot \frac{\partial^2}{\partial y^2}$$

$$P_z^2 = \frac{-h^2}{4\pi^2 m} \cdot \frac{\partial^2}{\partial z^2}$$

The expression on the L.H.S of equation represent a definite physical quantity i.e. kinetic energy of the particle while the equation on the R.H.S represents represents a symbol for the mathematical operation .The quantity on L.H.S of equation 1 is called Hamiltonian in classical mechanics while the in quantum mechanics, the operator within the square bracket of equation **2** on L.H.S is

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called the Hamiltonian operator represented by symbol $\hat{H}$ The compact form of Schrodinger equation is given by

$$\hat{H}\,\psi = E.\,\psi$$

Where H = Hamiltonan operator = $\frac{-h^2}{8\pi^2 m}\left(\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2} + V\right)$

Q.18) State and explain the postulates of quantum mechanics.

Ans. The Schrodinger wave equation describes the wave nature of the moving particle.There are different methods of using the wave equation so as to obtain the quantitative values of dynamic variables such as momentum, energy etc.In the new quantum mechanics, such values of the variables are obtained quickly without fully solving the wave equation using the postulates of quantum mechanics.They are as follows:

1.**Postulate I:**

To every system, a function is defined which is a function of all the variables of the system. Such a function is called as the state function of the system.

Explanation: The state function is represented by ψ .It may be real or complex. and should be single valued, continuous and finite.It must be a function of all variables of the system including time if necessary.

If q_1 ,q_2 ,q_3--------q_n denotes the dynamic variables for different particles of the system,then

State function Ψ (q_1 ,q_2 ,q_3--------q_n)

The state function is a creation of quantum mechanics. Einstein suggested that the probability of finding the system in a given region of space is proportional to Ψ^2 if Ψ is real and $\Psi\Psi^*$ .This leads to the condition of normalisation whose condition is

$$\int \Psi^2 .d\tau = 1 \quad \text{or} \quad \int \Psi\Psi^* \, d\tau = 1$$

A wavefunction that satisfies the above condition is called normalised wave function.

Postulate II:

For every dynamic variable of the system, an operator for the variable is defined by quantum mechanics.

Eg.

Dynamic variable	Quantum mechanical operator
Position(x)	x
Position(r)	r
Momentum along x axis	$p_x = \frac{h}{2\pi r} \frac{\delta}{\delta x}$
K.E of the particle	$\frac{-h^2}{8 \pi^2 m} . \nabla^2$

Postulate III:

The possible values of any dynamic variable of a system (energy, angular momentum) are given by eigen values 'a' in operator equation

$$A.\psi = a\,\psi$$

where A is operator corresponding to that physical quantity and ψ is a well behaved eigen function.

Postulate IV:

The average or expectation value of a variable of a system is given by

$$< a > \; = \frac{\int \Psi^* A \Psi d\tau.}{\int \Psi\Psi^* d\tau}$$

where A is an operator of the variable.

If the state function Ψ is normalised, then

$\int \Psi\Psi^* d\tau = 1$ therfore the above equation becomes

$$< a > \; = \int \Psi^* A \Psi d\tau$$

Postulate V:

If wave function (ψ) is physical system given at a certain instant (t), then its subsequent behaviour should be described as a derivative of wave function w.r.t time at that instant.

This relationship is given by $-\frac{ih}{2\pi} \frac{\partial\psi}{\partial t} (x, y, z, t) = H . \psi (x, y, z, t)$.

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