Wave Mechanics: Part – 1

Introduction:

The dynamical variables [position coordinates (r), linear momentum (p), angular momentum (L), magnetic moment (M), moment of inertia (I) etc.] in classical physics are not independent of one another and hence cannot be determined independently. If any two of these variables are known, the others can be successively estimated from suitable relations existing among them. Thus. Of we know some sets of quantities, the other quantities van be determined. We can choose number of subsets of independent variables from the set of all dynamical variables. There are large numbers of sets (compatible) whose number is restricted by Poisson brackets which are specific functions of dynamical variables.

A Poisson bracket is defined as - $\{u, v\} = \sum_k (\frac{\partial u}{\partial q_k} . \frac{\partial v}{\partial p_k} - \frac{\partial u}{\partial p_k} . \frac{\partial v}{\partial q_k})$;

Where u, v are functions of the generalized position (q_k) and momentum (p_k) co-ordinates.

In quantum mechanics, the Poisson brackets are replaced by commutator brackets. A commutator bracket is defined as $[u, v]_c = uv - vu$

These two brackets are related by the relation $\{u, v\}_p = \frac{1}{i\hbar}[u, v]_c$; where $\hbar = h/2\pi$ = Reduced Planck's constant.

The properties of commutator brackets are identical with those of Poisson's brackets, e.g.

$$[A, (B+C)] = [A, B] + [A, C] \text{ and } [A, cB] = c[A, B] \text{ where c is a constant.}$$

A quantity G is said to commute with the operator H if

$$[G, H] = GH - HG = 0$$

The quantities occurring in the commutators are functions of positions and momenta co-ordinates and are called **Observables**, as they can be measured by performing suitable experiments on the system.

A pair of observables is called **Compatible** if they can be measured simultaneously. However, they will be called **Incompatible** if they can bot be measured simultaneously.

Two incompatible observables do not commute mutually e.g. position and momentum of a particle.

Physical significance of wave function Ψ:

According to de Broglie theory, a beam of electrons behaves like a beam of photons. Thus the fundamental assumption in quantum mechanics is that the motion of particle can be represented by complex wave packet in space and time. This wave function for a material article can be represented by the real and imaginary part of a wave function of the form

$$\psi = \psi_0 e^{i(kx - \omega t)}; where\ k = \frac{2\pi}{\lambda} = propagation\ constant.$$

The wavelength λ for a standing wave corresponding to the electron in n^{th} orbit of radius r is given by

$$2\times\pi\times r = n\times\lambda \quad \text{i.e.} \quad \mathbf{\lambda = (2\times\pi\times r)/n}$$

The energy E of a particle wave is not spread out over the entire extent of the wave as in case of classical waves but is localized with the particle. Still the accompanying wave is essential to account for the phenomena of interference and diffraction. The fact that the phase velocity of de Broglie waves is greater than the velocity of light in vacuum does not constitute any violation of the postulates of special theory of relativity as no energy is transmitted at the phase velocity.

In classical mechanics, the square of the wave amplitude associated with an electromagnetic radiation gives the measure of radiation intensity. Similarly, in quantum mechanics, the wave function Ψ associated with the motion of a particle must correspond to some physically observable property of the particle. Actually, Ψ includes all the relevant information about the behavior of the particle i.e. describes it completely. In other words, if the wave function of a particle is known, then the result of any experiment carried out on it can be obtained mathematically. For a system of non-interacting particles, Ψ^2 may be regarded as a measure of the density of the particles.

Further, the magnitude of Ψ is large in a region where the probability of finding the particle is large, and its magnitude is small in a region where the probability of finding the particle is small. Thus **Ψ may be regarded as a measure of the probability of finding a particle around a particular point.** Since the probability is real and positive whereas Ψ is complex (in general), the position probability density is considered as $\Psi\,\Psi^* = |\Psi|^2$, Ψ* being the complex conjugate of Ψ. So $|\Psi|^2 dv$ gives the probability of finding the particle in a small element of volume dv at a certain position. Hence $|\Psi|^2$ may be called the probability function. Since the particle must be somewhere in the space, the integration of $|\Psi|^2$ over the entire space must be unity. $\therefore \int |\psi|^2\, dv = 1$

Such wave functions are called normalized wave function. For every system which is bound, every wave function must satisfy this relation. The numerical co-efficient of Ψ that normalizes it must be independent of time so that it may satisfy Schrodinger equation. Any solution of Schrodinger equation is such that $\int |\psi|^2\, dv$ taken over the entire space is independent of time.

Postulates of Quantum Mechanics:

The basic postulates of quantum mechanics are:

[1] Every dynamical state of a particle can be represented by a wave function which includes all that can be known about the particle.

[2] The principle of superposition is valid for wave functions which represents physically admissible states.

[3] The wave functions of a system are normalized functions.

[4] For every physically measurable or observable quantity of a system (position, velocity, momentum, energy etc.), there must have a corresponding linear Hermitian operator in quantum mechanics.

   a. If $A(C\Psi) = CA\Psi$ i.e. if A commutes with C and $A(\Psi_1 + \Psi_2) = A\Psi_1 + A\Psi_2$, then A is a linear operator.

   b. If $\int (A\psi)^* \psi\, dv = \int \psi^* (A\psi)\, dv$, then A is a Hermitian operator.

[5] The commutator bracket of two operators in quantum mechanics is related to the classical Poisson bracket by the relation $[L, M]_c = i\hbar\{l, m\}_p$; where L, M are the Hermitian operators corresponding to the classical observables l, m.

[6] The only possible values for a physical property are the eigen values of the corresponding operator equation involving a well behaved eigen function.
   a. The eigen values of a Hermitian operator are real
   b. The eigen values of a Hermitian operator are orthogonal, if they correspond as distinct eigen.

[7] The eigen values of an operator corresponding to any physical property constitute a complete set.

[8] If a large number of measurements are made on any physical property (variable) represented by an operator A belonging to a system, characterized by the wave function Ψ, then the average or **<u>expectation value</u>** of the variable is given by, $\lambda = \frac{\int \psi^*(A\psi)dv}{\int \psi^*\psi dv}$; where A is an operator.

[9] The necessary and sufficient condition for a real expectation value is that the dynamical variable must be represented by a Hermitian operator.

[10] The time development of a wave function Ψ is given by,

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi;$$ where H is the Hamiltonian operator.

This equation is known as **<u>Schrodinger equation</u>**.

[11] Schrodinger wave equation gives the behavior of a wave function both in space and time.

[12] The wave function and its partial derivatives must be finite, continuous and single values for all values of x, y, z, and t.

<u>Operators and Operand:</u>

- The expression $\frac{d\psi}{dx}$ may be regarded to consist of two constituents – the operator $\frac{d}{dx}$ and operand Ψ.
- The unit operator is that operator which does not alter the operand.
- The zero operator is that operator which vanishes the operator.

<u>Eigen Function and Eigen Value:</u>

If the operator α operates on the operand Ψ and yields the value λΨ, where λ is called the <u>Eigen Value</u> of the operator α corresponding to the operand Ψ, called <u>Eigen Function</u>.

i.e. if $\alpha\Psi = \lambda\Psi$; then Ψ → Eigen Function; α → operator; λ → Eigen Value.

<u>Simultaneous Eigen Function:</u>

If two operators have two different eigen values corresponding to a single eigen function, then this eigen function is said to be a simultaneous eigen function of those operators. If Ψ is a simultaneous eigen function of two operators α and β, then -- $\alpha\Psi = m\Psi$ and $\beta\Psi = n\Psi$.

Here m and n are the eigen values of the operators α and β respectively corresponding to the eigen function Ψ.

Now, $\alpha\Psi = m\Psi$; => $\beta(\alpha\Psi) = \beta(m\Psi) = m(\beta\Psi) = mn\Psi$; => $\beta\alpha\Psi = mn\Psi$ ------- (1)

Also, $\beta\Psi = n\Psi$; => $\alpha(\beta\Psi) = \alpha(n\Psi) = n(\alpha\Psi) = nm\Psi$; => $\alpha\beta\Psi = mn\Psi$ ------- (2)

Comparing (1) and (2);

$\alpha\beta\Psi = \beta\alpha\Psi$ => $(\alpha\beta - \beta\alpha)\Psi = 0 = 0.\Psi$

Hence $(\alpha\beta - \beta\alpha)$ is an operator of the eigen function Ψ whose eigen value is zero. This is the condition so that Ψ may be a simultaneous eigen function of the operators α and β.