Wave Mechanics

* Inadequacy of classical mechanics :-

classical mechanics is obeyed by macroscopic particles such as planets and rigid bodies. since, the microscopic particles such as electron, proton, atoms and molecules show wave particle duality.

In Bohr's theory, electron is treated as particle But a/c to de-Broglies theory, electron has dual character both as a material particles as well as wave. The dual character of an electron however obey quantum mechanics a key feature of which is the quantisation of energy and angular momentum.

In classical mechanics, the state of the system is defined by specifying all the force acting and all the position and velocity of the particles. while, Heisenberg Uncertainty principle comes into the picture. It show that simultaneous specification of position & momentum is impossible for a microscopic particles.

classical mechanics allows us to predict the exact path taken by the particles of the system. while quantum mechanics gives only the probability of finding the particles at various locations in space.

In quantum mechanics, the state of the system is defined by the state function or Wave function 'ψ'.

If the electron behave as a wave, there must be a wave equation to describe their behaviour. Erwin Schrodinger gave a wave equation to describe the wave behaviour of electrons in atoms and molecules. The Schrodinger wave equation for an electron wave propagating in three dimensional space is given as -

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

Where,

ψ = Wave function

E = Total energy

V = Potential energy

m = mass of electron

h = plank's constant.

$\frac{\partial^2\psi}{\partial x^2}$, $\frac{\partial^2\psi}{\partial y^2}$ & $\frac{\partial^2\psi}{\partial z^2}$ are the double differential of ψ w.r.t x, y & z respectively.

*. Basic Postulates of Quantum Mechanics :-

There are some unique sets of rules which provides mathematical language to quantum mechanics. These are known as postulates of quantum mechanics.

These are —

Postulates – I

The state of a microscopic system is described in terms of a function of position co-ordinate & time called Wave function 'ψ'.

Postulates – II

Their correspond a quantum mechanical operator to every observable quantities as :-

Physical quantities	operators
(a) Position	$\hat{x}$ (Linear Co-ordinates) $\hat{r}$ (Spherical Co-ordinates)
(b) Momentum	$\hat{P}_x \left(\frac{h}{2\pi i} \cdot \frac{\partial}{\partial x}\right)$ $\hat{P}_y \left(\frac{h}{2\pi i} \cdot \frac{\partial}{\partial y}\right)$ $\hat{P}_z \left(\frac{h}{2\pi i} \frac{\partial}{\partial z}\right)$
(c) Kinetic energy (K.E)	$\frac{-h^2}{8\pi^2 m} \cdot \nabla^2$
(d) Potential energy (P.E)	V
(e) Total energy ($E = K.E + P.E$)	$\frac{-h^2}{8\pi^2 m} \cdot \nabla^2 + V$

Postulates - III

The possible values of any physical quantities of a system are given by the eigen value 'a' in the operator equation as:

$$\hat{A}\,\psi = a\,\psi$$

where, $\hat{A}$: an operator

ψ : Wave function

a : Eigen value

This equation is called as eigen value equation.

In Hamiltonian form the above equation is written as:

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

where, $\hat{H}$: Hamiltonian operator

E : Eigen value

ψ : Wave function.

Postulates - IV

The average value (or expection value) $\langle A \rangle$ of an observable 'A' corresponding to the operator $\hat{A}$ is obtained from the relation

$$\langle A \rangle = \int_{-\infty}^{+\infty} \psi^* \hat{A} \psi \, d\tau$$

If ψ is normalised $\hat{A}$ is the operator of A.

Postulates - V

A physically observable quantity can be represented by a Hermitian operator. An operator $\hat{A}$ is said to be Hermitian of it satisfies the following conditions.

$$\int \psi_i^* \hat{A} \psi_j \, dx = \int \psi_j \left(\hat{A} \psi_i\right)^* dx$$

Postulates - VI

The time dependent Schrodinger equation is given as -

$$\hat{H}\psi = \frac{ih}{2\pi}\frac{\partial\psi}{\partial t}$$

Since, this is a partial differential equation involving both position & time variable. It can be solved only be seperated it in to differential equation.

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