Quantum Mechanics (or Wave Mechanics)

Classical mechanics is obeyed by macroscopic particles such as planets & rigid bodies. However, since the microscopic particles such as electrons, protons, atoms & molecules show wave particle duality, they do not obey the classical mechanics. However, they obey quantum mechanics & key feature of which is the quantization of energy & angular momentum.

Towards Quantum Mechanics:- There are certain properties of matter which could not be explained by classical mechanics & lead to formulation of new model these are:

1) Dual behaviour of matter 2) Heisenberg uncertainity principle

1) **De Broglie Hypothesis (Dual nature of matter & Radiation) wave-particle duality:-** It was suggested by Newton that light is a stream of particles which are photons (or Corpuscles) i.e. light has particle nature. However, this concept failed to explain the phenomenon of interference & diffraction which could be explained only if light is considered as wave nature. But at the same time, it was observed that black body radiation & photo electric effect could be explained only if light is considered to have particle. Hence finally it has been concluded that light has dual behaviour.

Louis-de Broglie, advanced the idea that like photons, all material particles such as electron, proton, atom, molecules, a stone or an iron ball (i.e. microscopic as well as macroscopic objects) also possess dual character. The wave associated with a particles is called a matter wave or de Broglie wave.

The de Broglie Relation:- In case of a photon, if it is assumed to have wave character, its energy is given by

$$E = h\nu \quad \text{—(1)} \quad [\text{according to Planck's quantum theory}]$$

where ν is frequency of wave & h is Planck's constant.

If the photon is supposed to have particle character its energy is given by

$$E = mc^2 \quad [\text{according to Einstein eqn.}] \quad \text{—(2)}$$

where m is the mass of photon & c is velocity of light.
from (1) & (2)

$$h\nu = mc^2$$

But $\nu = c/\lambda$

$$\therefore \; h \cdot \frac{c}{\lambda} = mc^{\cancel{2}}$$

or $$\lambda = \frac{h}{mc}$$

de Broglie pointed out that the above eqn. is applicable to any material particle. The mass of photon is replaced by mass of material particle & velocity c of photon is replaced the velocity v of material particle. Thus for any material particle like electron we may write:

$$\boxed{\lambda = h/mv}$$

or $$\boxed{\lambda = h/p}$$

$p = mv$ = momentum of particle.

Significance of de-Broglie eqn.:— Although the de-Broglie eqn. is applicable to all material objects but it has significance only in case of microscopic particles. This can be explained as follows:
Consider a ball of mass 0.1 kg moving with a speed of $60\ ms^{-1}$. From de Broglie eqn. the wavelength of associated wave $= \frac{h}{mv} = \frac{6.62 \times 10^{-34}\ kg\ m^2 s^{-1}}{0.1\ kg \times 60\ ms^{-1}} \simeq 10^{-34}\ m$

Hence this wavelength is too small for ordinary observation.
On the other hand, an electron with a rest mass equal to $9.11 \times 10^{-31}\ kg \simeq 10^{-30}\ kg$ moving at the same speed would have a wavelength $= \frac{6.62 \times 10^{-34}\ kg\ m^2 s^{-1}}{10^{-30}\ kg \times 60\ ms^{-1}} \simeq 10^{-5}\ m$ or 10^5 Å
which can be easily mesured experimentally.

Since we come across macroscopic objects in our everyday life, therefore de Broglie relationship has no significance in everyday life. This is why we do not observe any wave nature associated with the moving running car or cricket ~~batter~~. ball etc.

Comparison of classical mechanics with Quantum mechanics :-

Classical Mechanics	Quantum Mechanics
i) It deals with macroscopic particles	i) It deals with microscopic particle.
ii) It is based on Newton's laws of motion	ii) It takes into account Heisenberg's uncertainity principle & de Broglie concept of dual nature of matter.
iii) It is based on Maxwell's electromagnetic wave theory according to which any amount of energy may be emitted or absorbed continuously	iii) It is based on Planck's quantum theory according to which only discrete values of energy are emitted or absorbed
iv) The state of a system is defined by specifying all the forces acting on the particles as well as their positions & velocities (momenta). The future state can then be predicted with certainity	iv) It gives probabilities of finding the particles at various locations in space.

The Postulates of Quantum Mechanics:- The following are the postulates of quantum mechanics

1) The physical state of a system at time t is described by wave function $\psi(x,t)$, ~~this function is single valued, continuous & finite throughout the space.~~

2.) The wave function $\psi(x,t)$ & its first & second derivatives $\partial\psi(x,t)/\partial x$ & $\partial^2\psi(x,t)/\partial x^2$ are continuous, finite & single valued for all values of x. Also the wave function $\psi(x,t)$ is normalized i.e.

$$\int_{-\infty}^{\infty} \psi^*(x,t)\,\psi(x,t)\,dx = 1$$

where ψ^* is complex conjugate of ψ formed by replacing i with $-i$ wherever it occurs in the function ψ ($i=\sqrt{-1}$)

3.) A physically observable quantity can be represented by Hermitian operator. An operator $\hat{A}$ is said to be Hermitian if it satisfies the following condition:

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

where ψ_i & ψ_j are the wave functions representing the physical state of quantum system i.e. a particle, an atom or a molecule.

4.) The allowed values of an observable A are the eigen values a_i, in the operator eqn.

$$\hat{A}\psi_i = a_i \psi_i$$

The above eqn. is known as eigen value eqn. where a_i is an eigen value.

5.) The average value (or, the expectation value) $\langle A \rangle$ of an observable A, corresponding to operator $\hat{A}$ is obtained by relation

$$\langle A \rangle = \frac{\int_{-\infty}^{\infty} \psi^* \hat{A} \psi \, dx}{\int_{-\infty}^{\infty} \psi^* \psi \, dx}$$

[If ψ is normalized then $\int \psi^*\psi\, dx = 1$]

6.) To each observable quantity in classical mechanics, like, position, velocity, momentum, energy etc. there corresponds a certain mathematical operator in quantum mechanics the nature of which depends ~~on~~ upon the classical expression for the observable quantity. Some classical mechanical observable & their corresponding quantum mechanical operators are given in following Table

Classical variable (observables) Name	Symbol	operators symbol	operation
Position	x	$\hat{x}$	Multiplication by x
Position squared	x^2	$\hat{x}^2$	Multiplication by x^2
Momentum	p_x	$\hat{p}_x$	$-i\frac{h}{2\pi}\frac{\partial}{\partial x} = -i\hbar\frac{\partial}{\partial x}$
	p	$\hat{p} = -i\hbar\left[i\frac{\partial}{\partial x}+j\frac{\partial}{\partial y}+k\frac{\partial}{\partial z}\right]$	(taking derivative w.r.t. x & multiply by $-i\hbar$)
Momentum squared	p_x^2	$\hat{p}_x^2$	$-\frac{h^2}{4\pi^2}\frac{\partial^2}{\partial x^2} = -\hbar^2\frac{\partial^2}{\partial x^2}$ (taking double derivative w.r.t. x & multiply by $-\hbar^2$)
Kinetic Energy	$T_x = \frac{p_x^2}{2m}$ K	$\hat{T}_x$ $\hat{K} = \frac{-\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right]$	$-\frac{h^2}{8\pi^2 m}\frac{\partial^2}{\partial x^2} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
Potential energy	$V(x)$	$\hat{V}(x)$	Multiplication by $\hat{V}(x)$
Total energy	$E = T_x + V(x)$	$\hat{H}$ $-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right]+V(x,y,z)$	$-\frac{h^2}{8\pi^2 m}\frac{\partial^2}{\partial x^2}+V(x)$

1.7.0

Num:- Show that e^{ax} is an eigen function of the operator d/dx & find the corresponding eigen value. Show that e^{ax^2} is not an eigenfunction of d/dx

Ans:- In first case $\psi = e^{ax}$ $\therefore \frac{d\psi}{dx} = \frac{d}{dx}(e^{ax}) = ae^{ax} = a\psi$

Hence e^{ax} is an eigen function of d/dx & its eigen value is a

In IInd case $\psi = e^{ax^2}$

$$\therefore \frac{d\psi}{dx} = \frac{d}{dx}(e^{ax^2}) = \cancel{x.e^{ax^2}} \cancel{\frac{d}{dx}(ax^2)}\, e^{ax^2}\frac{d}{dx}(ax^2)$$

$$= 2ax\,e^{ax^2} = 2ax\psi$$

Thus the result obtained is not a constant factor multiplied with ψ but a variable factor $2ax$ multiplied with ψ.
Hence e^{ax^2} is not an eigenfunction of d/dx

Num:- Justify whether the function $\cos ax$ is an eigen function of a) d/dx b) d^2/dx^2. What is the corresponding eigenvalue if any?

Sol :- a) Here $\psi = \cos ax$ $\therefore$ $\frac{d\psi}{dx} = \frac{d}{dx}(\cos ax)$

$= -a \sin ax$

Hence $\cos ax$ is not an eigen function of d/dx

b) $\frac{d^2\psi}{dx^2} = \frac{d^2}{dx^2}(\cos ax) = \frac{d}{dx}\left(\frac{d}{dx}\cos ax\right)$

$= \frac{d}{dx}(-a \sin ax) = -a^2 \cos ax = -a^2 \psi$

Hence $\cos ax$ is an eigen function of d^2/dx^2 with eigen value $= -a^2$

Num :- Find commutators of the operators for momentum & position, the two conjugate properties of Heisenberg's uncertainity principle.

Sol :- $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$, $\hat{x} = x$

Let $\psi(x)$ be the operand

$\therefore [\hat{p}_x, \hat{x}]\psi = [p_x x - x p_x]\psi$

$= \left[-i\hbar \frac{\partial}{\partial x} \cdot x - x\left(-i\hbar\frac{\partial}{\partial x}\right)\right]\psi$

$= -i\hbar \frac{\partial}{\partial x}(x\psi) - x(-i)\hbar\frac{\partial \psi}{\partial x}$

$= -i\hbar\psi - \cancel{i\hbar x\frac{\partial\psi}{\partial x}} + \cancel{i x\hbar\frac{\partial\psi}{\partial x}} = -i\hbar\psi$

or $[\hat{p}_x, \hat{x}] = -i\hbar$

Hence momentum & position do not commute therefore they cannot be mesured simultaneously