<u>Introduction of quantum mechanics</u>

Quantum mechanics is a fundamental theory in physics that describes the behavior of matter and energy at the smallest scales, typically at the level of atoms, molecules, and subatomic particles. Quantum mechanics deals with systems where classical physics no longer applies, revealing the underlying rules governing the quantum world. In the case of subatomic particles moving at hery high speed, classical physics will not yield correct results when we try to measure the dynamic parameteres related to the system. Quantum mechanics is emerged in the early 20th century to resolve inconsistencies in classical physics. With the help of quantum mechanics it is possible to explain phenomena such as Blackbody Radiation, Photoelectric Effect and Atomic Spectra.

Key accepts of Quantum Mechanics

Quantum mechanics is able to explain below mentioned properites exhibited by subatomic particles which could not be explained by classical physics.

a. **Wave-Particle Duality**

- One of the most important concepts in quantum mechanics is that particles, such as electrons and photons, exhibit both **wave-like** and **particle-like** behavior.
- Waves associated with particle in motion are called matter waves or de Broglie waves. The wavelength associated with mattern waves is called de Broglie waves is $\boldsymbol{\lambda = h/p}$ where h is Plank's constant (h = 6.626×10^{-34} J/s) where h is the Plank's constant and p the momentam of the particle.

The properties of matter waves are the following

- Matter waves are considered as probability amplitude wave
- matter waves exhibit diffraction phenomenon
- it does not require a medium of propogation
- matter waves obey superpositon principle

b. Quantization

- Many properties of particles, such as energy, momentum, and angular momentum, are **quantized**, meaning they can only take on discrete values rather than any value in a continuous range.

- For example, in an atom, electrons can only occupy certain energy levels, and they transition between these levels by absorbing or emitting specific amounts of energy (quanta).

c. Superposition

- A fundamental feature of quantum systems is the ability of a particle to exist in a **superposition** of states. This means that until it is measured, a particle can exist in multiple states simultaneously.
- This principle is famously illustrated in **Schrödinger's cat** thought experiment, where a cat is both alive and dead in a quantum superposition until observed.

d. Wavefunction (Ψ)

- The **wavefunction** (Ψ) is a central concept in quantum mechanics that mathematically describes the quantum state of a system. It contains all the information about a particle’s possible positions, momenta, and other properties.
- The square of the wavefunction’s magnitude ($|\Psi|^2$) gives the **probability density** of finding a particle in a specific location or state.

e. Heisenberg Uncertainty Principle

- The **uncertainty principle**, formulated by Werner Heisenberg, states that it is impossible to precisely measure both the position (x) and momentum (p) of a particle simultaneously: $\Delta x \cdot \Delta p \geq h/2\pi$ This principle arises because particles in quantum mechanics do not have definite positions and momenta until measured.

3. Schrödinger Equation

- The **Schrödinger equation** is the fundamental equation of motion in quantum mechanics that describes how the quantum state (wavefunction) of a system evolves over time. This equation can be solved for various physical systems (e.g., atoms, particles in a box) to determine the allowed energy levels and behavior of the particles.

Formulate Time dependent Schrodinger equation from solution of plane wave

Schrödinger equation is a the fundamental equation in quantum mechanics.

It can be derived by considering the plane wave equation and combining it with of Energy-frequency relation & De-Broglie expression.

Let us consider a free particle (free from all external forces), moving in the positive X-direction and the corresponding wave function, which contains all the information about the motion is given by,

$$\Psi(x,t) = Ae^{i(kx - \omega t)}$$

Where, k= - Wave vector. = 2pi/lamda

$\omega = 2\pi\gamma$ - Angular frequency.

According to De-Broglie expression, $P = \frac{h}{\lambda}$; $P = \frac{h\,.\,2\pi}{\lambda\,.\,2\pi} = \frac{h\,.\,2\pi}{2\pi\,.\,\lambda\,.} = \hbar k$

$$\boxed{k = \frac{P}{\hbar}} \quad - (2)$$

According to Energy-Frequency rel., $E = h\upsilon$; $E = h\upsilon\,\frac{2\pi}{2\pi} = \frac{h}{2\pi}\,2\pi\upsilon = \hbar\omega$

$$\boxed{\omega = \frac{E}{\hbar}} \quad - (3)$$

Substitute equation (2) and (3) in eq (1) we get,

$$- \quad \boxed{\Psi(x,t) = Ae^{\frac{i}{\hbar}((Px - Et)}} \quad - (4)$$

Differentiating equation (4) twice with respect to 'x'

$\frac{i}{\hbar}((Px - Et)$

$$- \quad \boxed{E\,\Psi(x,t) = i\hbar\,\frac{\partial\Psi}{\partial t}} \quad - (6)$$

Consider the particle of mass 'm' moving with a velocity 'v', then the total energy 'E' of the system,

$$E = \text{Kinetic Energy} + \text{Potential Energy}$$

$$E = \frac{1}{2}mv^2 + V$$

$$E = \frac{mv^2}{2}\,\frac{m}{m} + V = \frac{m^2v^2}{2m} + V;$$

$$E = \frac{p^2}{2m} + V$$

Multiply on both side with 'Ψ(x,t)'

$$\boxed{E\,\Psi(x,t) = \frac{p^2}{2m}\,\Psi(x,t) + V\,\Psi(x,t)} \quad - (7)$$

Substituting **(4), (5) & (6)** in **(7)** we get,

$$\boxed{i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + \mathbf{V}\,\Psi}$$

is the 1- Dimensional time dependent Schrodinger wave equation.

- The Three dimensional Time- dependant Schrodinger equation can be written as,

$$\boxed{i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2\Psi + \mathbf{V}\,\Psi}$$

Where $\nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$ called Laplace's operator