Method of Quantum Mechanics.

* Introduction of ~~Quantum~~ Classical Quantum Mechanics.

-) The classical mechanics which deals with the matter of micro scopic phenomenon. These phenomenon are described by Newton's laws of motion. The second law of motion is widely used in macroscopic ~~Hence~~ phenomenon. Hence this laws is known as fundamental law of Newtonian mechanics. But classical mechanics could not explain the phenomenon like

1) The stability of atoms
2) Observed spectrum of black body radiation
3) Specific heat capacity at low temprature
4) The several phenomena like photo electric effects, Compton effect, Raman effect, plasma state, emmission of $\underbrace{\alpha, \beta}_{\text{particle}}, \underbrace{\gamma}_{\text{ray}}$ etc.

These phenomenon are explained by hypothesis of planck's, Bohr's postulates etc under the limitation. These theory proposed by them led to development of quantum mechanics such quantum mechanics is called ~~[illegible]~~ old quantum mechanis.

* Defficiency of Quantum Mechanics.

1) The Bohr's Theory explains well spectrum of monoelectronic Hydrogen, singally ionized He-atom, but it fails to explain the spectrum of the simplest multi-electron atom. For example: He

2) The most serious criticisms of the old quantum theory is that it is intellectually unsatisfied that is it is not a unified or general theory.

It deals with microscopic particles of a well defined path by uncertainity principle which is not possible.

3) This theory can be applied only to periodic system for example: harmonic oscillator, circular motion etc. but there are many imp physical system that are not periodic

These deficiencies help to develop the new quantum theory whose fundamental principle is wave function (eqn)

$\sin\theta - i\cos\theta$
$= e^{-i\theta}$

* wave equation (wave function) :-

→ The wave equation of the progressive wave at any instant of time 't' is given by :-

$$y = a\sin(\omega t - kx)$$

where,
a = amplitude , k = wave number $= \frac{2\pi}{\lambda}$

It can be written in the exponentially form as

$$y = a e^{-i(\omega t - kx)} \text{ ——— (i)}$$

$$E = h\nu$$
$$= \frac{h}{2\pi} \times 2\pi\nu$$
$$= \hbar\omega \Rightarrow \omega = \frac{E}{\hbar}$$

and $\lambda = \frac{h}{p}$

For x-axis

$$\lambda = \frac{h}{p_x}.$$

$$p_x = \frac{h}{\lambda}$$

$$= \frac{h}{2\pi} \times \frac{2\pi}{\lambda}$$

$$= \hbar k$$

$$\text{or } k = \frac{p_x}{\hbar}$$

Using value of k and ω in eqⁿ i)

$$y = a e^{-i\left(\frac{E}{\hbar} t - \frac{p_x}{\hbar} x\right)} \quad \text{—— ii)}$$

~~Then~~ This eqⁿ can be represected by a function $\psi(x,t)$

$$\therefore \psi(x,t) = a e^{-i\left[\frac{E}{\hbar} t - \frac{p_x}{\hbar} x\right]}$$

$$= a e^{\frac{-i}{\hbar}\left[Et - p_x x\right]}$$

$$= a e^{\frac{i}{\hbar}\left[p_x x - Et\right]}$$

$r = \hat{i}\hat{j}\hat{k}\,(x, y, z)$

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This is called wave function of particle in ~~x~~x-co-ordinate. In 3-dimension it can be written as

$$\psi(r,t) = a\, e^{\frac{i}{\hbar}[pr - Et]}$$

$r = (x, y, z)$

This is the fundamental wave eqn in terms of wave function. for new Quantum Mechanics.

quantum Mechanical Operator

* Introduction:-

→ In classical mechanics, energy and momentum can be expressed in terms of co-ordinate of a particle whereas in quantum mechanics, energy and momentum cannot be expressed in terms of co-ordinate of a particle to avoid a violation of uncertainity principle.
Hence to obtain the information of a quantum mechanical ~~part~~ particle, an operator is ~~introducted~~ introduced. The quantum mechanical operator is defined as a function which indicates an operation to be performed over a space of physical state to that of another.

$\frac{p_x}{\hbar}$

In order to introduce an operator a equation of form is given by

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

is known as eigen value equation where $\hat{A}$ is quantum mechanical operator

ψ is wave function (eigen function)

$a \rightarrow$ eigen value

[In german, eigen means proper]

→ There are two basic types of quantum mechanical operator

1. Momentum operator
2. Energy operator

(1) Momentum Operator:—

⇒ We have,

wave function of free quantum particle,

$$\psi = A e^{-\frac{i}{\hbar}[Et - P_x x]}$$

for +ve x-axis —i)

Taking derivative of eqn i) with respect to x.

$$\frac{\partial \psi}{\partial x} = \frac{\partial\, A e^{-\frac{i}{\hbar}[Et - P_x x]}}{\partial x}$$

$$\frac{\partial \psi}{\partial x} = A\left(\frac{-i}{\hbar}\right)(-P_x)\, e^{\frac{-i}{\hbar}[Et - P_x x]}$$

$$= \frac{iP_x}{\hbar}\psi$$

or $$P_x\psi = \frac{\hbar}{i}\frac{\partial \psi}{\partial x} = \frac{i\hbar}{i^2}\frac{\partial \psi}{\partial x} = -i\hbar\frac{\partial \psi}{\partial x}.$$

$$\therefore \quad P\psi = -i\hbar\frac{\partial \psi}{\partial x}$$

$$P \rightarrow -i\hbar\frac{\partial}{\partial x}$$

$$\therefore \quad \hat{P} \longrightarrow -i\hbar\frac{\partial}{\partial x}$$ for x-axis

This is momentum operator

(2) Energy operator

we have,

$$\varphi = a e^{-\frac{i}{\hbar}[Et - p_x]} \quad \text{---(i)}$$

Taking derivative wrt ~~to~~ time,

$$\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial t}\left(a e^{-\frac{i}{\hbar}(Et - p_x x)}\right)$$

$$\frac{\partial \psi}{\partial t} = a\left(\frac{-i}{\hbar}\right) E \left[e^{-\frac{i}{\hbar}(Et - p_x x)}\right]$$

or, $$\frac{\partial \psi}{\partial t} = \psi\left(\frac{-i}{\hbar}\right) E$$

or; $$E\psi = -\frac{\hbar}{i}\frac{\partial \psi}{\partial t}$$

$$= \frac{-i\hbar}{i^2}\frac{\partial \psi}{\partial t}$$

$$= i\hbar\frac{\partial \psi}{\partial t}$$

Hence $$E \longrightarrow i\hbar\frac{\partial}{\partial t}$$

This is called energy operator.
This shows that there is association of energy with operator $i\hbar \frac{\partial}{\partial t}$.

* Schrondinger wave equation's

Introduction:-
→ Schrondinger wave eqn is a fundamental wave eqn in terms of variable wave function ψ which describes the ~~proces~~ motion of quantum mechanical particle same as Newton's second law of motion does in classical mechanics. There are two types of schrondinger wave eqns:-

(1) Time dependent Schrondinger wave eqn

(2) Time independent Schrondinger wave eqn.

1) Time dependent :-

Inorder to derive the time dependent schrondinger wave eqn. consider a particle has well defined momentum and energy.

The wave function associated with motion of free particle in terms of momentum and energy is given by

$$\psi = Ae^{\frac{-i}{\hbar}[Et - P_x x]} \quad \text{— i)}$$

for +ve X-axis,

Taking derivative of ψ wr to x,

$$\frac{\partial \psi}{\partial x} = A\left(\frac{-i}{\hbar}\right)(-P_x)\, e^{\frac{-i}{\hbar}(Et - P_x x)}$$

$$= \frac{i P_x}{\hbar}\psi$$

Again taking derivative of $\frac{\partial \psi}{\partial x}$ wr to x

$$\frac{\partial^2 \psi}{\partial x^2} = \left[\frac{i P_x}{\hbar}\right]^2 \psi = \frac{-P_x^2}{\hbar^2}\psi$$

or $$P_x^2 \psi = -\hbar^2 \frac{\partial^2 \psi}{\partial x^2} \quad \text{— ii)}$$

Now,

Taking derivative ψ w.r.to t, From eqn i)

$$\frac{\partial \psi}{\partial t} = A\left(\frac{-i}{\hbar}\right) \times E\, e^{\frac{-i}{\hbar}[Et - p_x x]}$$

$$= \frac{-iE}{\hbar}\psi$$

$$E\psi = \frac{-\hbar}{i}\frac{\partial \psi}{\partial t}$$

$$= \frac{-i\hbar}{i^2}\frac{\partial \psi}{\partial t} = i\hbar\frac{\partial \psi}{\partial t} \quad \text{— ii)}$$

The total Energy of free particle

$$E = \text{total KE} + \text{PE}$$

$$E = \frac{p^2}{2m} + V \quad \text{— iii}$$

Multiplying by ψ on both sides,

$$E\psi = \frac{p_x^2\psi}{2m} + V\psi \quad \text{— iv}$$

Now using eqn i) and ii) in eqn iv

$$\therefore i\hbar\frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi$$

or, $\frac{i\hbar \partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V \right) \psi$

This is 1-D time dependent schrondinger wave eqn.

Let $H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V$ is called Hameltenion operator

Hence,

$$\therefore \boxed{\frac{i\hbar \partial \psi}{\partial t} = H\psi}$$

This is another form of 1-D time dependent schrondinger wave eqn.

2) Time independent :-

It is found that in many situations potential V acting on the particle does not depend on time and varies only with its position. For this condition time independent form of Schrondinger wave eqn is applicable.

In order to derive time independent SWE a particle has well defined momentum and energy can be given by wave function ψ as :-

$$\psi = Ae^{\frac{-i}{\hbar}[Et - Px]}$$

along X-axis

Taking derivative of ψ wrt x,

$$\frac{\partial \psi}{\partial x} = A\left(\frac{-i}{\hbar}\right) - Px \, e^{\frac{-i}{\hbar}[Et - Px]}$$

$$= \frac{iP_x \psi}{\hbar}$$

Taking derivative of $\frac{\partial \psi}{\partial x}$ wrt x,

$$\frac{\partial^2 \psi}{\partial x^2} = \left[\frac{iP}{\hbar}\right]^2 \psi = \frac{-P^2}{\hbar^2}\psi$$

$$P^2\psi = \frac{-\hbar^2 \partial^2 \psi}{\partial x^2} \quad \text{———} \; 2)$$

-P

Total Energy of free particle is given by

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

using eq^n i) in eq^n ii)

$$E\psi = \frac{p^2\psi}{2m} + V\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi$$

or $$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi - E\psi = 0$$

or, $$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}\left[E - V\right]\psi = 0 \quad \text{— ii)}$$

This is time independent SWE

In three dimension. It can be written as

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{2m}{\hbar^2}\left[E - V\right]\psi = 0$$

or $$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi + \frac{2m}{\hbar^2}\left[E - V\right]\psi = 0$$

since $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \nabla^2$ – Laplacean operator as Nebla

∇^2 Laplacean

$$\nabla^2 \psi + \frac{2m}{\hbar^2}[E - V]\psi = 0$$ Hame

$$\left[H = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V \right]$$

$$\nabla^2 \psi + \frac{2m}{\hbar^2} E\psi - \frac{2m}{\hbar^2} V\psi = 0$$

or

$$\frac{2m}{\hbar^2} E\psi = -\nabla^2\psi + \frac{2m}{\hbar^2} V\psi$$

or

$$E\psi = \frac{-\hbar^2}{2m}\nabla^2\psi + V\psi$$

$$= \left(\frac{-\hbar^2}{2m}\nabla^2 + V\right)\psi$$

$$\boxed{E\psi = H\psi}$$

$\therefore$ $H = \frac{-\hbar^2}{2m}\nabla^2 + V$ is a Hamelttaneon operator.

This is time independent SWE in ~~ϕ~~ 3D. in terms of Hamiltonian operator

* Schrondinger wave eqn of free particle.

we have,

$$\bar{\nabla}^2\psi + \frac{2m}{\hbar^2}\left[E - V\right]\psi = 0 \quad \text{--- (1)}$$

For free particle $V = 0$

Hence eqn (1) reduces to

$$\bar{\nabla}^2\psi + \frac{2m}{\hbar^2}\left[E\right]\psi = 0$$

This is SWE for free particle

* Physical significance of wave function (ψ)