QUANTUM MECHANICS

Introduction :-

Quantum mechanics is the science of very small. It explain the behaviour of matter & its interaction with energy on the scale of atomic & subatomic particles. Quantum mechanics is the foundation of several related disciplines including nanotechnology, condensed matter physics, Quantum mechanics, structural biology, particle physics and electronics.

For example :-

Uncertainity principle of quantum mechanics means that the more closely one pins down one measurement (such as position of particle the less accurate another complementary measurement pertaining to same particle such as its speed) must become.

Another example of quantum mechanics is "**entanglement**".

QUANTUM MECHANICS

Defination:- "Study of relation of EMR with matter is called quantum mechanics."

Postulates of Quantum mechanics:-

There are four postulates of quantum mechanics.

(i) Operator theorem
(ii) Eigen value theorem.
(iii) Expectation theorem.
(iv) Time dependent Schrodinger wave Equation.

★ **Operator theorem:-** "To every measurable physical quantity of a system, their corresponds an operator."

It has four types.

- linear operator
- Vector operator
- Laplacian operator
- Hamiltonian operator.

* Eigen value theorem :-

"If result of operation of an operator of function results is a some function with some numerical value

(i) $\frac{d}{dx} e^{x} = 1e^{x}$ (ii) $\frac{d}{dx} e^{ax} = ae^{ax}$

here a is numerical value

* Expectation theorem :-

If so many measurements are made on some system (function), then some expected value from eigen function in term of eigen values are calculated as.

$$A\psi = \lambda\psi \implies \lambda = \frac{\hat{A}\psi}{\psi}$$

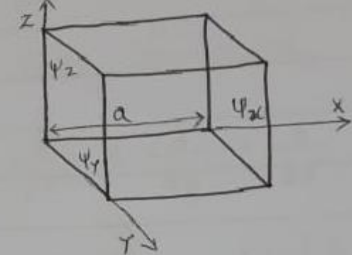
$$\lambda = \frac{\hat{A}\psi\psi^*}{\psi\psi^*} \implies \langle\lambda\rangle = \frac{\hat{A}\int_{-\infty}^{+\infty}\psi\psi^*}{\int\psi\psi^*}$$

* Time dependent Schrodinger wave Equation:-

In 1926, Schrodinger give thesis on wave mechanics and give some mathematical equation called schrodinger equation by joining two wave functions, two possibilities are these (i) Normalization (ii) Orthogonality

Schrodinger's wave Equation for a particle in three dimensions:-

Explanation:-



Consider a particle in three dimensional box of length a. The potential energy of particle will be the function of three coordinates. The PE inside the box is **zero** and at boundary and outside of the box, it will be infinity.

Schrodinger wave equation for a particle in three dimension can be written as :-

$$\nabla^2\psi_{xyz} + \frac{8\pi^2 m}{h^2}(E-V)\psi_{xyz} = 0 \quad \text{——— (1)}$$

Potential energy inside the box is zero

Hence, $V = 0$

Now equation (1) become as.

$$\nabla^2 \psi_{xyz} + \frac{8\pi^2 m}{h^2} E \psi_{xyz} = 0 \quad \text{——— (2)}$$

ψ_{xyz} is the wave function of particle moving in three dimension.

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad \text{——— (3)}$$

Put value of ∇^2 in Eq (2).

$$\frac{\partial^2}{\partial x^2}(\psi_{xyz}) + \frac{\partial^2}{\partial y^2}(\psi_{xyz}) + \frac{\partial^2}{\partial z^2}(\psi_{xyz}) + \frac{8\pi^2 m}{h^2} E \psi_{xyz} = 0 \quad \text{— (4)}$$

$$\psi_{xyz} = \psi_x \psi_y \psi_z \quad \text{—— (abc).}$$

Now equation (4) become as:

$$\psi_y \psi_z \frac{\partial^2 \psi_x}{\partial x^2} + \psi_x \psi_z \frac{\partial^2 \psi_y}{\partial y^2} + \psi_x \psi_y \frac{\partial^2 \psi_z}{\partial z^2} + \frac{8\pi^2 m}{h^2} E \psi_x \psi_y \psi_z = 0 \quad \text{— (5)}$$

On dividing both sides of Eq (5) by $\psi_x \psi_y \psi_z$.

$$\frac{1}{\psi_x}\frac{\partial^2 \psi_x}{\partial x^2} + \frac{1}{\psi_y}\frac{\partial^2 \psi_y}{\partial y^2} + \frac{1}{\psi_z}\frac{\partial^2 \psi_z}{\partial z^2} + \frac{8\pi^2 m}{h^2} E = 0 \quad \text{— (6)}$$

Multiply on both side of Eq (6) by $\frac{h^2}{8\pi^2 m}$, so that constant with E can be removed.

$$\frac{h^2}{8\pi^2 m}\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2} + \frac{h^2}{8\pi^2 m}\frac{1}{\psi_y}\frac{\partial^2\psi_y}{\partial y^2} + \frac{h^2}{8\pi^2 m}\frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2} + E_{xyz} = 0 \quad (7)$$

and we Know that

$$E_{xyz} = E_x + E_y + E_z.$$

By putting the value of E_{xyz} in Eq (7).

$$\frac{h^2}{8\pi^2 m}\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2} + \frac{h^2}{8\pi^2 m}\frac{1}{\psi_y}\frac{\partial^2\psi_y}{\partial y^2} + \frac{h^2}{8\pi^2 m}\frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2} + E_x + E_y + E_z = 0$$

$$\frac{h^2}{8\pi^2 m}\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2} + \frac{h^2}{8\pi^2 m}\frac{1}{\psi_y}\frac{\partial^2\psi_y}{\partial y^2} + \frac{h^2}{8\pi^2 m}\frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2} = -E_x - E_y - E_z \quad (8)$$

By separating the corresponding parts of equation (8)

$$\frac{h^2}{8\pi^2 m}\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2} = -E_x \quad 9(a)$$

$$\frac{h^2}{8\pi^2 m}\frac{1}{\psi_y}\frac{\partial^2\psi_y}{\partial y^2} = -E_y \quad \text{—— } 9(b)$$

$$\frac{h^2}{8\pi^2 m}\frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2} = -E_z \quad \text{—— } 9(c)$$

Equation 9(a) can be written as.

$$\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2} = -\frac{8\pi^2 m}{h^2} E_x.$$

$$\frac{\partial^2\psi_x}{\partial x^2} = -\frac{8\pi^2 m}{h^2} E_x \psi_x.$$

$$\frac{\partial^2\psi_x}{\partial x^2} + \frac{8\pi^2 m}{h^2} E_x \psi_x = 0.$$

Let,

$$\frac{8\pi^2 m}{h^2} E_x = \text{constant} = K^2$$

Then Eq (9a), 9(b) and 9(c) can be written as:

$$\frac{\partial^2 \psi_x}{\partial x^2} + K^2 \psi_x = 0 \quad \text{——— } 10(a)$$

$$\frac{\partial^2 \psi_y}{\partial y^2} + K^2 \psi_y = 0 \quad \text{——— } 10(b)$$

$$\frac{\partial^2 \psi_z}{\partial z^2} + K^2 \psi_z = 0 \quad \text{——— } 10(c)$$

Equation 10(a)(b)(c) is called as second order differential equation.

Solution Of Schrodinger Wave Equation In three dimension:-

By solving Eq 10(a) second order differential equation and has solution in exponential solution as :-

$$\psi_x = Ae^{mx} \quad \text{——— } (11)$$

Basically, x represents the direction of wave function & m. A are constants

Put value of Equation (11) in Eq 10(a):
we get

$$\frac{\partial^2}{\partial x^2}(Ae^{mx}) + K^2 Ae^{mx} = 0$$

$$Am^2e^{mx} + K^2Ae^{mx} = 0$$

$$Ae^{mx}(m^2+K^2) = 0.$$

Hence

$$Ae^{mx} \neq 0.$$

So,

$$m^2 + K^2 = 0 \quad \text{——— (a)}$$

This Equation is called Auxillary Equation

$$m^2 = -K^2$$

$$m^2 = -1(K^2)$$

$$m^2 = i^2K^2$$

$$m = \sqrt{i^2K^2}$$

$$m = \pm iK \quad \text{——— (12)}$$

Put Value of m in Eq(11)

$$\psi_x = Ae^{\pm ikx} \quad \text{——— (13)}$$

Eq (13) is exponential equation that contains two part. Real and imagenary part.

$$\psi_x = Ae^{ikx} \cdot e^{-ikx}$$

$$\psi_x = Ae^{ikx} + Be^{-ikx}$$

Following trignometric function are given as:

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

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

$$\psi_x = A[\cos(Kx) + i\sin(Kx)] + B[\cos Kx - i\sin(Kx)]$$

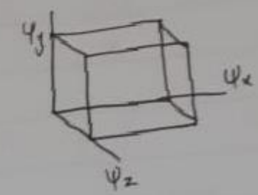
$$= \cos(Kx)[A+B] + i\sin(Kx)[A-B].$$

let,

$$[A+B] = D \quad \& \quad i[A-B] = C$$

$$\psi_x = D\cos(Kx) + C\sin(Kx) \quad \text{——— (14)}$$

By applying boundary conditions on Eq(14)



(1) When $x = 0$ & $\psi x = 0$

$$0 = D\cos(k.0) + C\sin(k.0)$$

$$= D\cos 0^\circ + C\sin 0$$

$$= D(1) + 0$$

$$D = 0$$

Hence eq (14) become.

$$\psi_x = C\sin(kx) \quad \text{——} (15)$$

(2) When $x = a$ & $\psi x = 0$

Put 2nd condition in Eq (15)

$$0 = C\sin(ka)$$

This condition is true only if and only if

$$Ka = n\pi$$

$$K = \frac{n\pi}{a} \quad \text{——— (16)}$$

Put value of K in eq (15), we get.

$$\psi_x = C \sin \frac{n\pi x}{a} \quad \text{——— 17(a)}$$

$$\psi_y = C \sin \frac{n\pi y}{a} \quad \text{——— 17(b)}$$

$$\psi_z = C \sin \frac{n\pi z}{a} \quad \text{——— 17(c)}$$

Determination Of Value Of "C":-

In order to calculate the maximum overlapping, we shall apply condition of **normalization**.

$$\int_0^a \psi_x \psi_x^* \, d\psi = 1 \quad \text{——— (18)}$$

Substituting value of ψ_x by putting eq 17(a) to (18)

$$\int_0^a C \sin \frac{n\pi x}{a} \; C \sin \left(\frac{n\pi x}{a}\right) dx = 1$$

$$\int_0^a C^2 \sin^2\left(\frac{n\pi x}{a}\right)dx = 1$$

$$C^2\int_0^a \sin^2\left(\frac{n\pi x}{a}\right)dx = 1 \quad \text{------ (19)}$$

As we know that

$$\therefore \quad 2\sin^2\theta = 1 - \cos 2\theta$$

$$\sin^2\theta = \frac{1-\cos 2\theta}{2}$$

So,

$$\sin^2\left(\frac{n\pi x}{a}\right) = \frac{1-\cos\left(\frac{2n\pi x}{a}\right)}{2} \quad \text{------ (20)}$$

Put eq 20 in eq (19).

$$C^2\int_0^a \frac{1-\cos\left(\frac{2n\pi x}{a}\right)}{2}dx = 1$$

$$\frac{C^2}{2}\left[\int_0^a\left(1-\cos\frac{2n\pi x}{a}\right)dx\right] = 1$$

$$\frac{C^2}{2}\left[\int_0^a dx - \int_0^a \cos\frac{2n\pi x}{2}dx = 1\right.$$

As we know,

$$\therefore \int \cos \frac{2n\pi x}{a}\, dx = \frac{\sin 2n\pi x/a}{2n\pi/a}$$

So we get the values as

$$\frac{c^2}{2}\left[(a-0) - \int_0^a \left(\frac{a}{2n\pi}\right) \cdot \sin \frac{2n\pi x}{a}\Big|\right] = 1$$

$$\frac{c^2}{2}\left[a - \frac{a}{2n\pi}\left(\sin \frac{2n\pi a}{a} - \sin \frac{2n\pi 0}{a}\right)\right] = 1$$

and we know that

$$\frac{c^2}{a}\left[(a) - 0\right] = 1$$

$\sin n\pi$, $\sin 0$, $\sin 2\pi = 0$.

$$\frac{c^2}{2} a = 1$$

$$c^2 a = 2$$

$$c^2 = 2/a$$

$$\boxed{c = \sqrt{2/a}}$$

Put value of C in eq 17(a), 17(b)
Eq 17(c).

$$\psi_x = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \quad \text{—— 21(a)}$$

$$\psi_y = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi y}{a}\right) \quad \text{—— 21(b)}$$

$$\psi_z = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi z}{a}\right) \quad \text{—— 21(c)}$$

Put value of ψ_x, ψ_y and ψ_z in Eq (abc), we get.

$$\psi_{xyz} = \psi_x \psi_y \psi_z$$

$$\psi_{xyz} = \sqrt{\frac{2}{a}} \cdot \sqrt{\frac{2}{a}} \sqrt{\frac{2}{a}} \sin^3\left(\frac{n\pi x}{a}\right)^3 \quad \text{—— (22)}$$

This is the wave equation of particle in three dimension.

Properties:-

- The general form of solution of

Schrodinger wave equation is.

$$\psi(x,t) = Ae^{i(Kx-\omega t)} = A[\cos(Kx-\omega t) + i\sin(Kx-\omega t)]$$

Which also describe a wave moving in the x-direction. In general, amplitude may also complex. This is called **wave function** of particle.

- The wave function is also not restricted to being real. We know that sin term has an imagenary number. Only physically measurable quantities must be real. These include the probability, momentum and energy.

Results :-

- It is used in calculation of total wave function.
- It is used to calculate total energy

"Total Energy Of Particles Entrapped In Three Dimensional Box"

We Know that

$$K^2 = \frac{8\pi^2 m}{h^2} E_x \quad \text{------} (1)$$

Also

$$K = \frac{n\pi}{a} \quad \text{------} (2)$$

Taking its Square

$$K^2 = \frac{n^2\pi^2}{a^2} \quad \text{------} (3)$$

Comparing eq (1) & (3)

$$\frac{8\pi^2 m}{h^2} E_x = \frac{n^2\pi^2}{a^2}$$

$$E_x = \frac{n_x^2 h^2}{8a^2 m} \quad \text{------} (4)$$

So, this equation represent total energy along x-axis.

Where h = Plonk's constant

Similarly we can found that

$$E_y = \frac{n_y^2 h^2}{8a^2 m} \text{ ——— } (5)$$

$$E_z = \frac{n_z^2 h^2}{8a^2 m} \text{ ——— } (6)$$

We also know that

$$E_{xyz} = E_x + E_y + E_z.$$

Thus by putting the values we can find total energy of particles entrapped in 3-D box.

$$E_{xyz} = \frac{h^2}{8ma^2} (n_x^2 + n_y^2 + n_z^2)$$

This shows $\boxed{\text{Degeneracy}}$ exists of different quantum states having same energy is Known as degeneracy.

DEGENRACY ⇒ Same energy & different position

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