Contents:

Quantum Mechanics

Introduction:

Quantum mechanics is the science of very small. It explains 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 is "entanglement".

Quantum Mechanics

Definition :-
"Study of relation of EMR with matter is called Quantum mechanics"

Postulates of Quantum mechanics :-

There are four postulate 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, there 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 in a same 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.

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

$$\lambda = \frac{\hat{A}\psi\psi^*}{\psi\psi^*} \Rightarrow \langle\lambda\rangle = \frac{\hat{A}\int\psi\psi^*}{\int\psi\psi^*}$$

- **Time dependent Schrodinger wave Equation:-**

In 1926, Schrodinger give thiesis on wave mechanics and give some mathematical equation called Schrodinger equation. By joining two wave function, two possibilities are there. (i) Normalization (ii) Orthogonality.

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

Explanation:-

Consider a particle in three dimensional box of length a. The potential energy of particle will be the function of three coordinates. The P.E 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:-

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

Potential energy inside the box is zero. Hence, $V=0$

Now equation (1) become as.

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

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

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

put value of ∇^2 in Eq(2).

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

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

Now equation (4) become as:

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

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

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

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

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

and we know that,

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

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

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

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

By separating the corresponding parts of equation (8)

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

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

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

Equation 9(a) can be written as.

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

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

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

Let

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

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

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

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

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

Eq 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:-

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

$$A m^2 e^{mx} + k^2 A e^{mx} = 0$$

$$A e^{mx} (m^2 + k^2) = 0$$

$\therefore \frac{\partial}{\partial x} \times \frac{\partial}{\partial x} e^{mx}$

$\frac{\partial}{\partial x} (m e^{mx})$

$m^2 e^{mx}$.

hence, $A e^{mx} \neq 0$.

So, $m^2 + k^2 = 0$ — (a)

This Equation is called **Auxillary Equation:**

$$m^2 = -k^2$$

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

$$m^2 = i^2 k^2$$

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

$$m = \pm ik \quad \text{— (12)}$$

Put value of m in Eq (11).

$$\boldsymbol{\psi_x = A e^{\pm ikx}} \quad \textbf{— (13)}$$

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

$$\psi_x = A e^{ikx} . e^{-ikx}.$$

$$\psi_x = A e^{ikx} + B e^{-ikx}.$$

Following trignometric function are given as:

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

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

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

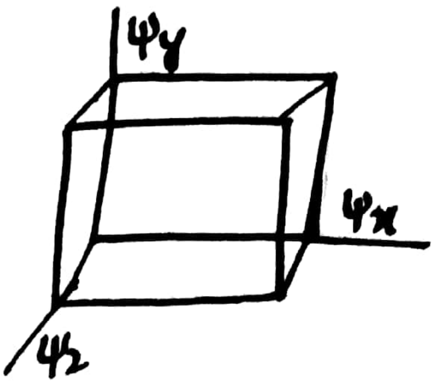
$$= \cos(kx)[A+B] + i\sin(kx)[A-B]$$

Let.

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

$$\psi_x = D\cos(kx) + C\sin(kx) \text{ --- (14).}$$

By applying boundary conditions on Eq(14).



(1) when $x = 0$ & $\psi_x = 0$.

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

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

$$= D(1) + 0$$

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$D = 0$.

hence Equation (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).

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

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

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

As we know that.

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

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

So, $\sin^2\left(\frac{n\pi x}{a}\right) = \frac{1-\cos\left(\frac{2n\pi x}{a}\right)}{2}$ ...... Eq(20)

Put Equation 20 in Eq(19).

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

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

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

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

$$\frac{C^2}{2}\left[1x\Big|_0^a - \Big|_0^a \frac{\sin 2n\pi x/a}{2n\pi/a}\right.$$

As we know,

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

So, we get the values as :-

$$\frac{c^2}{2}\left[(a-0) - \Big|_0^a \left(\frac{a}{2n\pi}\right) \cdot \sin \frac{2n\pi x}{a}\Big|\right] = 1$$

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

and we know that

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

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

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

$$c^2 a = 2$$

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

$$c = \sqrt{\frac{2}{a}}$$

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

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

Eq(abc) can be written as.

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

$$\psi_{xyz} = \sqrt{2/a} \cdot \sqrt{2/a} \sqrt{2/a} \sin\left(n\pi x/a\right).$$

$$\sin\left(\frac{n\pi y}{a}\right) \cdot \sin\left(\frac{n\pi z}{a}\right) \quad \text{--- } (22)$$

It 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 the **wave function of particle**.

- The wave function is also not restricted to being real. we know that sin term has an imaginary 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.

Calculation of total Energy:-

we have find the schrodinger wave equation in three dimension. Now, we calculate the total energy.

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

and we know that $$k = \frac{n\pi}{a} \quad \text{---} (2)$$

Taking square on both side of Eq (2), we get

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

By compareing Eq (1) & Eq (3).

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

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

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

$$\boxed{E_x = \frac{n^2{}_x h^2}{8ma^2}} \quad \text{---} (4)$$

It is the energy of particle along x-axis.
Similarly, we found that.

$$E_y = \frac{n_y^2 h^2}{8ma^2} \text{ ——— (v)}$$

$$E_z = \frac{n_z^2 h^2}{8ma^2} \text{ ——— (vi)}$$

hence total energy will be.

$$E_{xyz} = E_x + E_y + E_z \text{ ——— (vii)}$$

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

$$E_{total} = \frac{h^2}{8ma^2}\left(n_x^2 + n_y^2 + n_z^2\right) \text{ ——— (viii)}$$

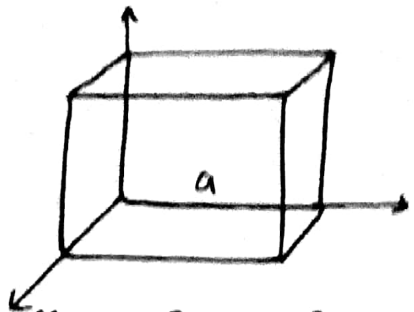
With the help of Eq(viii), we find total energy of particle entrapped in 3D box.

Factors upon which total Energy depend upon:-

(i) $E_{total} \propto \frac{1}{a^2}$

(ii) $E_{total} \propto \frac{1}{m}$

Hence these energy effect the structure of box.



Basically n_x, n_y, n_z depends upon principle Quantum number.

Minimum energy is called as **Ground energy**. we can calculate it if

$$n_x = n_y = n_z = 1$$

$$E_{total} = \frac{h^2}{8ma^2}(1^2+1^2+1^2).$$

$$\boxed{E_{total} = \frac{3h^2}{8ma^2}}$$

This is the Ground state Energy.

Definition:-

The lowest amount of energy a particle possess in 3D box. is known as Ground state energy.

Cases:

Case 1:-

Let if $n_x = 2$ & $n_y, n_z = 1$

So,

$$E_{total} = \frac{h^2}{8ma^2}(2^2+1^2+1^2)$$

$$= \frac{6h^2}{8ma^2}$$

Case 2:-

If $n_x = 1$, $n_y = 2$ & $n_z = 1$

then,

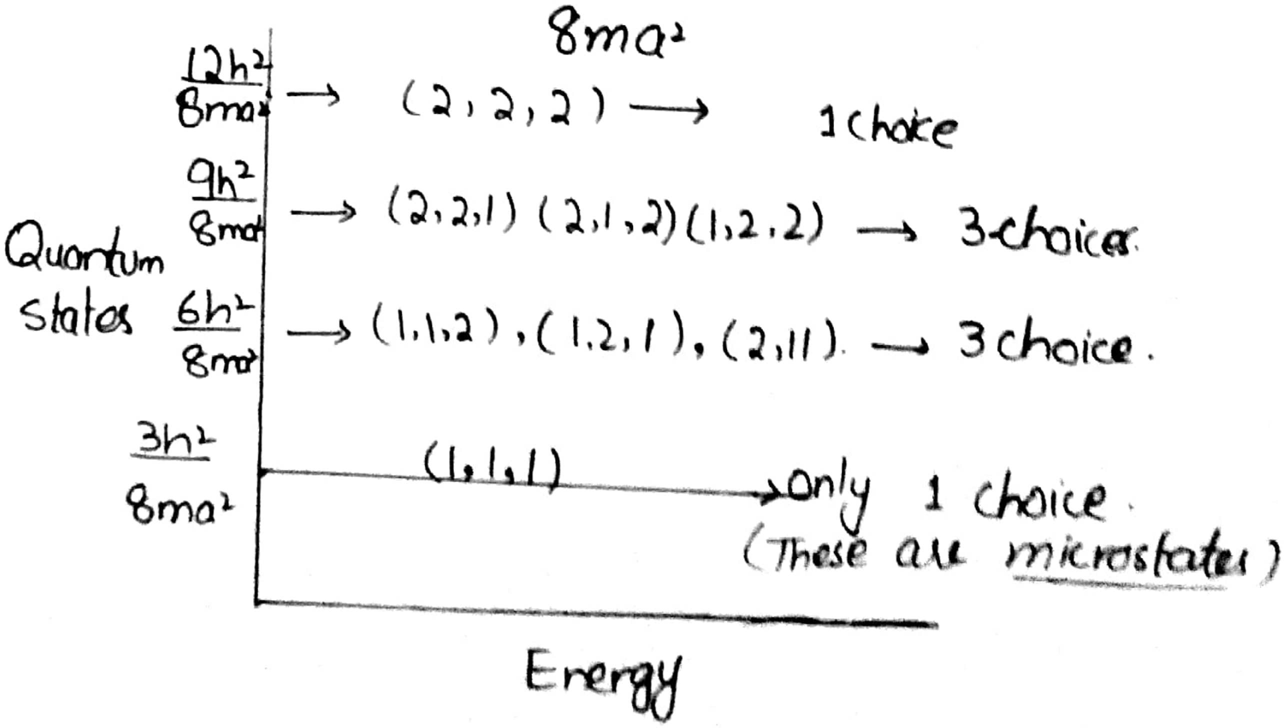
$$E_{total} = \frac{6h^2}{8ma^2}$$

Case 3:-

If $n_x = 1$, $n_y = 1$ & $n_z = 2$

then,

$$E_{total} = \frac{6h^2}{8ma^2}$$



Entropy :-

Entropy is the state of increasing number of microstats or Quantum States.

Degeneracy :-

The existance of distinct or different Quantum state having some energy is called degeneracy.

- **Microstates :-**

It is the state of energy possession.

- **Macrostates :-**

Number of ways of distribution of energy is called macrostates.