"CONTENTS"

"Wave Function"

Definition:-

A wave function in quantum physics is a Methematical description of Quantum state of an isolated Quantum System. The wave function is a Complex value Probability, amplitude and the Probabilities for possible results of measurements made on the system can be derived for it. The most common sysmbol for a wave function are the

Greek letter "ψ" or "Psi".

The wave function is the function of the degree of freedom, Corresponding to some maximal Set of Communicating Observables. The wave function can be derived from the Quantum state.

Types Of Wave Function:-

There are basically two types of wave function. But the third one also exists.

1- Normallized Wave function

2- Orthogonal Wave function.

3- Orthonormal Wave function.

"Differentiate Between Orthogonal And Normalized Wave Functions"

Time-Dependant Schrodinger Wave Equation:-

This is the Fourth Postulate of Quantum Mechanics. In 1926 Schrondinger give an Of Wave Mechanics.

Wave Function is a Kind of System Represented by "ψ" or "Psi". This "ψ" describes the Properties of a System. "ψ" is a complex number.

"Complex Number" consists of two Parts.

Exp:- Complex No:- Real + Imaginary

$$A = x + iy$$

$$\psi = a + ib$$

The conjugate of "ψ" is "ψ^*"

$$\psi^* = a - ib$$

Maximum Overlap of "ψ" and "ψ^*"

$$\int_{-\infty}^{+\infty} \psi \psi^* d\psi = 1$$ (Ideal Conditions are there)

$$\int_{-\infty}^{+\infty} \psi^2 d\psi = 1$$

Wave Functions are "Normalized".

Conditions for Normalization:-

$\Rightarrow$ When $\psi \psi^* d\psi$ becomes equal to 1, Then this is called the Conditions for "Normalization".

Sometimes, When $\psi \psi^* d\psi$ becomes equal to "Zero" then it is Known as "Orthogonality".

$$\int_{-\infty}^{+\infty} \psi \psi^* d\psi = 0$$

$$\Rightarrow \quad \psi \psi^* = a^2 + b^2$$

Normalization:-

$$\int_{-\infty}^{+\infty} \psi_x \psi_x^* = 1$$

$$\int_{-\infty}^{+\infty} \psi_x^2 dx = 1$$

When the Integral of the wave function time its Complex conjugate over the entire space available is equal to unity. Then this wave function is called "Normalized Wave Function". and this condition is called "Normalization."

Limits are extended from $-\infty$ to $+\infty$ and the Integral must be equal to unity. Since the particle must exist somewhere in that integral if it is to exist at all. For Three dimensions, we can write the above equation as:-

$$\int_{-\infty}^{+\infty} \psi^2 d\tau = 1 \qquad \therefore d\tau = dx, dy, dz$$

(small volume elements)

The square of the wave function is proportional to the probability of finding the particle in the given volume element. All values of wave function ψ are not acceptable. The acceptable values are

Those which have been normalized by multiplying the function by a proper constant. If ψ is the solution of wave equation multiplication by a constant value A then it will give $A\psi$ (A into ψ), which is also a solution. It means that means that the

$$\int_{-\infty}^{+\infty} \psi \psi^* \, dx\,dy\,dz \text{ is proportional to probability.}$$

The probability of certainity is unity. Thus the probability of electron being in the volume element is unity. The maximum probability of existance of something in space should be unity, no matter what is the exact distribution in that region of space may be.

USE OF NORMALIZATION:-

⇒ Normalization is a process of reducing redundancies of Data in database.

⇒ Essentialy, Normalizing the wave function means you find the exact form that ensure the probability that the particle is found somewhere in space is equal to 1.

⇒ The process of Normalization also has a constant known as:

"Constant Of Normalization"
denoted by
"C"

Normalization And Constant Of Normalization:-

Let's Consider the three wave functions:

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

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

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

In these three equations "C" is Known as the "Constant of Normalization."

Determination Of Value Of "C":-

We Know that for the maximum overlap, we should apply the "Conditions for Normalizations."

i.e

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

If we put the value of ψ_x from equ (a) to equ (A) then,

$$A \Rightarrow \int_0^a C\sin\frac{(n\pi x)}{a} \cdot C\sin\frac{(n\pi x)}{a}\, dx = 1 \quad \text{— (B)}$$

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

$$c^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx = 1 \quad \text{—} (B) \quad \therefore \int \sin\theta = -\cos\theta$$

We Know that

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

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

So:-

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

Put the value from (C) to equ (B)

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

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

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

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

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

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

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

As We Know:-

$$\sin 0, \sin 2\pi, \sin 3\pi, \sin n\pi = 0$$

So we get:-

$$\frac{C^2}{2}a - 0 = 1$$

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

$$C^2 a = 2$$

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

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

This "C" is Known as "Constant of Normalization"
So by putting the value of "C" in eqn (a),(b),(c)
we get:-

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

$$\psi_Y = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi Y}{a}\right)$$

$$\psi_z = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi z}{a}\right)$$

By putting values of $\Psi_x \cdot \Psi_y \cdot \Psi_z$ in equation

$$\Psi_{xyz} = \Psi_x \cdot \Psi_y \cdot \Psi_z$$

$$\Psi_{xyz} = \sqrt{\frac{2}{a}} \cdot \sqrt{\frac{2}{a}} \cdot \sqrt{\frac{2}{a}} \cdot \sin\left(\frac{n\pi x}{a}\right) \cdot \sin\left(\frac{n\pi y}{a}\right) \cdot \sin\left(\frac{n\pi z}{a}\right)$$

This equation gives Total wave function of particle moving in 3-D box.

How To Normalize a Wave Function:-

Normalizing a wave function Just means multiplying it by a constant to ensure that the sum of the probabilities for finding the particle equals to 1.

Mathematically:- This means integrating $\Psi^*(x)\Psi(x)dx$ over all space should equal to 1

$$\int_{-\infty}^{+\infty} \Psi^*_{(x)} \Psi_{(x)}\, dx = 1$$

Example # 01:-

The $n = 2$ State for a particle in a box of length $L = 1$

Unnormalized $= \Psi_x = \sin(2\pi x)$

Normalized $= \Psi_x = \sqrt{2}\sin(2\pi x)$

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Unnormalized —— Probability sum to 0.5

Normalized —— Probability sum to 1.0

As we know:- $\psi(x) = \sin(2\pi x)$

let's check is it Normalized?

$$\int_{-\infty}^{+\infty} \psi^*(x)\, \psi(x)\, dx = \int_0^1 [\sin(2\pi x)][\sin(2\pi x)]\, dx$$

$$= \int_0^1 \sin^2(2\pi x)\, dx$$

$$= \frac{1}{2\pi} \int_0^{2\pi} \sin^2 u\, du$$

$$= \frac{1}{2\pi} \int_0^{2\pi} \sin^2 u\, du$$

$$= \frac{1}{2\cancel{\pi}} \cancel{\pi}$$

$$= \frac{1}{2} \Rightarrow \text{Not Normalized}$$

To convert it into a Normalized wave function we multiply it by a constant "A"

$$\psi(x) = A \sin(2\pi x)$$

What value of A will make it Normalized.

$$\int \psi^*(x)\, \psi(x)\, dx = \int_0^1 [A \sin(2\pi x)][A \sin(2\pi x)]\, dx$$

$$= A^2 \int_0^1 \sin^2(2\pi x)\, dx$$

$$= \frac{A^2}{2} = 1 \Rightarrow \text{If Normalized}$$

$$\frac{A^2}{2} = 1 \Rightarrow A^2 = 2$$

$$A = \sqrt{2}$$

And our Normalized Wave function is:-

$$\psi_{(x)} = \sqrt{2}\sin(2\pi x)$$

Example # 02:-

Normalize a wavefunction for a Particle in a box of length L given by:

$$\psi_{(x)} = x(L-x)$$

$$\int \psi^*_{(x)}\psi_{(x)}dx = \int_0^L [Ax(L-x)][Ax(L-x)]dx$$

$$= A^2\int_0^L x^2(L-x)^2 dx$$

$$= A^2\int_0^L x^4 - 2Lx^3 + L^2x^2 dx$$

$$= A^2\left[\frac{x^5}{5} - \frac{2Lx^4}{4} + \frac{L^2x^3}{3}\right]_{x=0}^{x=L}$$

$$= \frac{A^2L^5}{30} = 1 \quad \text{If Normalized.}$$

$$= A^2 = \frac{30}{L^5}$$

$$= A = \sqrt{\frac{30}{L^5}}$$

So:- Our final Normalized Wavefunction is:-

$$\psi_x = \sqrt{\frac{30}{L^5}}\,x(L-x)$$

"ORTHOGONALITY"

Definition:-

There are many acceptable solutions to Schrodinger Wave Equation for a particular System.

$$\hat{H}\Psi = E\Psi$$

Each wave function has a corresponding energy value E. For any two wave functions Ψ_n and Ψ_m corresponding to the energy values E_n and E_m. The Following condition must be fulfilled.

$$\int_{-\infty}^{+\infty} \Psi_n \Psi_m \, dx = 0$$

Such a condition is called condition of "Orthogonality Of Wavefunction". The two functions Ψ_n and Ψ_m are said to be orthogonal to each other.

From this it implies that the Orthogonality is a relationship between two wavefunctions and a single wave function itself can not be labbled as "orthogonal." They must be orthogonal with respect to some other wavefunction.

There is an exception in Orthogonality. when 2 or more wavefunctions corresponds to same energy level. Then these are called "degenarate levels." Wave function for degenarate level are not always Orthogonal to one another but they are orthogonal to all other wave functions that are solutions of some wave Equation.

In vector form the term "Orthogonal" means "Perpendicular". For perpendicular vectors, their dot Product is Zeero. Orthogonal means scalar product = 0. For functions, Scalar product is the integral of the product of functions values. For instance, "sin and cos" are two "Orthogonal Functions." Often used to describe "Waves".

Derivation for Orthogonal Wave function:-

If an electron exists in the two Quantum states corresponding to two wave functions (ψ_l, ψ_m) and fulfill the condition.

$$\int_{-\infty}^{+\infty} \psi_l \cdot \psi_m \, d\tau = 0 \quad -(1)$$

Let consider that

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

let $n = l, m$ in eq (2a)

$$\psi_l = \sqrt{\frac{2}{a}} \sin\left(\frac{l\pi x}{a}\right) \quad -(2b)$$

$$\psi_m = \sqrt{\frac{2}{a}} \sin\left(\frac{m\pi x}{a}\right) \quad -(2c)$$

In the case of 3-D box put (2b) and (2c) in (1)

① ⟹ $$\int_0^a \left[\sqrt{\frac{2}{a}} \sin\left(\frac{l n\pi x}{a}\right) \cdot \sqrt{\frac{2}{a}} \sin\left(\frac{m\pi x}{a}\right)\right] dx = 0$$

$$\frac{2}{a} \int_0^a \left[\sin\left(\frac{l\pi x}{a}\right) \cdot \sin\left(\frac{m\pi x}{a}\right)\right] dx = 0$$

As we know:-

$$2\sin A \cdot \sin B = \cos(A-B) - \cos(A+B)$$

$$\frac{1}{a} \int_0^a \left[2\sin\left(\frac{l\pi x}{a}\right) \cdot \sin\left(\frac{m\pi x}{a}\right)\right] dx = 0$$

$$\frac{1}{a} \int_0^a \left[\cos\left(\left(\frac{l\pi x}{a}\right) - \left(\frac{m\pi x}{a}\right)\right) - \cos\left(\frac{l\pi x}{a} + \frac{m\pi x}{a}\right)\right] dx = 0$$

$$\frac{1}{a} \int_0^a \cos \frac{\pi x}{a}(l-m)\, dx - \frac{1}{a} \int_0^a \cos \frac{\pi x}{a}(l+m)\, dx = 0$$

$$\frac{1}{a} \frac{\sin \pi x (l-m)}{\frac{\pi}{a}(l-m)} \Bigg|_0^a - \frac{1}{a} \frac{\sin\left(\frac{\pi x}{a}\right)(l+m)}{\frac{\pi}{a}(l+m)} \Bigg|_0^a = 0$$

$$\frac{1}{a} \frac{a}{\pi(l-m)} \left[\frac{\sin(a)(l-m)}{a} - \frac{\sin(0)(l-m)}{a}\right] - \frac{1}{a} \frac{a}{\pi(l+m)} \left[\frac{\sin\pi(a)(l+m)}{a} - 0\right] = 0$$

$$\frac{1}{\pi(l-m)} \left[\sin\pi(l-m) - 0\right] - \frac{1}{\pi(l+m)} \left[\sin\pi(l+m) - 0\right] = 0$$

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If $l = 1$ then $m = 0, \pm 1$

for $(l-m)$

$$l - m = 1 - 0 = 1$$

$$l - m = 1 - (-1) = 2$$

$$l - m = 1 - (+1) = 0$$

for $(l+m)$

$$l + m = 1 + 0 = 1$$

$$l + m = 1 + (-1) = 0$$

$$l + m = 1 + (+1) = 2$$

This equation can be satisfied only, If 0, $\sin 1\pi$, $\sin 2\pi$ is equal to zero.

$$0, \sin 1\pi, \sin 2\pi = 0$$

Therefore it has been proved that both of the wave functions are orthogonal to each other.

So, the wave function that are the solution of "Schrodinger Wave Equation" are the "Orthogonal" to each other. And their product should be equal to zero.

Examples For Orthogonality:-

Show that

$$[1, \cos x, \sin x, \cos 2x \ldots\ldots]$$

for an orthogonal set on $[-\pi, \pi]$.

Example # 01:-

Show: $(1, \cos(nx)) = 0$

$$= \int_{-\pi}^{+\pi} \cos(nx)\,dx$$

$$= \frac{1}{n} \sin(nx) \Big|_{-\pi}^{+\pi}$$

$$= \frac{1}{n} \left[\sin(n\pi) - \sin(-n\pi)\right]$$

Both are multiple of π

So:-

$$\frac{1}{n}[0 - 0] = 0$$

So function $(1, \cos(nx))$ is orthogonal.

Example # 02:-

Show: $(1, \sin(nx)) = 0$

$$\int_{-\pi}^{\pi} \sin(nx)\,dx$$

$$= -\frac{1}{n} |\cos(nx)|_{-\pi}^{\pi}$$

$$= \frac{-1}{n}\left[\cos(n\pi) - \cos(-n\pi)\right] \quad \therefore \cos(-\theta) = \cos\theta$$

$$= \frac{-1}{n}\left[\cos(n\pi) - \cos(n\pi)\right]$$

$$= 0$$

Example # 03

Show:- $[\sin(nx), \sin(mx)] = 0 \quad n \neq m$

$$\int_{-\pi}^{\pi} \sin(nx) \cdot \sin(mx)\, dx$$

$\therefore \quad \sin A \cdot \sin B = \frac{1}{2}\left[\cos(A-B) - \cos(A+B)\right]$

So:-

$$= \int_{-\pi}^{\pi} \frac{1}{2}\left[\cos(nx - mx) - \cos(nx + mx)\right] dx$$

$$= \frac{1}{2}\int_{-\pi}^{\pi}\left[\cos(n-m)x - \cos(n+m)x\right] dx$$

$$= \frac{1}{2}\left| \frac{1}{n-m}\sin(n-m)x - \frac{1}{n+m}\sin(n+m)x \right|_{-\pi}^{\pi}$$

$$= \frac{1}{2}\left[\frac{1}{n-m}\underbrace{\sin(n-m)\pi}_{0} - \frac{1}{n+m}\underbrace{\sin(n+m)\pi}_{0}\right] - \left[\frac{1}{n-m}\underbrace{\sin(n-m)(-\pi)}_{0} - \frac{1}{n+m}\underbrace{\sin(n+m)(-\pi)}_{0}\right]$$

$$= 0$$

Because We Know that:-
sin (multiple of π) = 0

So the above equation becomes equal to "zero"

ORTHONORMAL WAVE FUNCTION:-

If $\psi_1^* \psi_2 = 1$ the the wave function is Normalized. If $\psi_1^* \psi_2 = 0$, then the wave function is the Orthogonal. If the Wave function is both orthogonal and Normalized then it is called "Orthonormal Wavefunction."

Condition For Orthonormality:-

$$\int_{-\infty}^{+\infty} \psi_n^* \psi_m \, d\tau = 1 \qquad \text{if } n = m$$

$$\int_{-\infty}^{+\infty} \psi_n^* \psi_m \, d\tau = 0 \qquad \text{if } n \neq m$$

The above relations can be combined as:

$$\int_{-\infty}^{+\infty} \psi_n^* \psi_m \, d\tau = \delta_{nm}$$

"δ_{mn}" called "Kronecker delta".

It can be defined as:

$$\delta_{nm} \begin{cases} 0 & \text{for } n \neq m \\ 1 & \text{for } n = m \end{cases} \quad \text{— (A)}$$

The Wave function that satisfied the condition (A) is called "ORTHONORMAL WAVE FUNCTION."