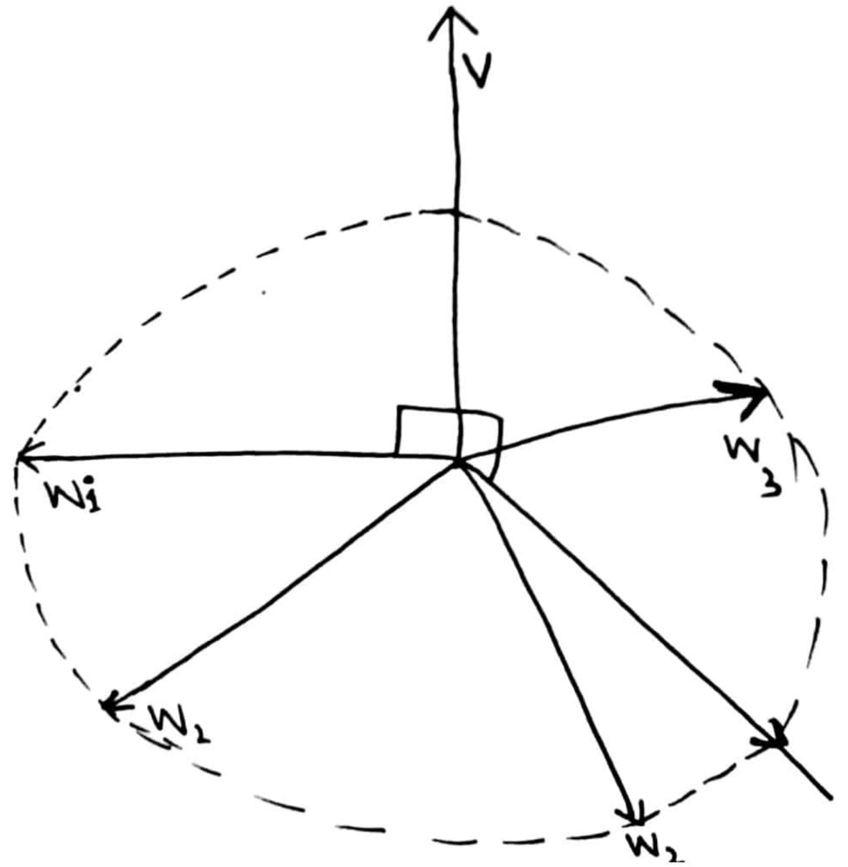
(Q.1)

Defference between orthogonal and Normalization wave function with example?

⇒ Orthogonal Wave function:

Defination:-

Means perpendicular. For perpandicular vector their dot product is zero wave function can be regardas vector in infinite dimensional linear vactor space to represent such vector we need an infinite dimensional space with orthogonal **basic** set of vactors.



Orthogonal Wave Function :-

Let us Consider wave function ψ and ϕ and $\psi^* \phi^*$

$$\int \psi^* \phi \, dv = 0$$ En → no degenrate

$E_n \neq E_n$

Proof

$$\hat{H}\psi_n = E_n \psi_n \longrightarrow (1)$$

$$\hat{H}\psi_m = E_m \psi_m \longrightarrow (2)$$

$$\int_{-\infty}^{\infty} \psi_m^* H \psi_n \, dv = \int \psi_n^* E_n \psi_n \, dv$$

$$= E_n \psi_m^* E_n \psi_n \, dv$$

$$= E_n \int \psi_m \psi_n^* \psi_n \, dv \longrightarrow (3)$$

$$\int_{-\infty}^{\infty} (H\psi_m^*) \psi_n \, dv = E_m \int \psi_m^* \, dv \longrightarrow (4)$$

$$\int (A\psi^*) \psi \, dv = \int \psi (A\psi) \, dv$$

$$E_m \int \psi_m^* \psi_m \, dv = E_n) \int \psi_m^* \psi_n \, dv$$

$$(E_m - E_n) \psi_m^* \psi_n \, dv = 0$$

$E_m \neq E_n$

$$\boxed{\int \psi_m^* \psi_n \, dv = 0}$$

If two wave function $\psi_1 + \psi_2$

$$\int \psi_1^* \psi_2 \, dv = \int \psi_1 \psi_2^* \, dv = 0$$

For Example :-

$\psi_1 = \sin x + \psi_2 = \cos$

$$\int_0^{2\pi} \sin x \cdot \cos x \, dx = 1/2 \int_0^{2\pi} 2 \sin x \cdot \cos x$$

$$1/2 \left[\cos 2x \right]_0^{2\pi}$$

$$1/2 \int_0^{2\pi} \sin 2x \, dx = 1/2 \left[\cos 2\cancel{x} \right]_0^{2\pi}$$

$\cos 2\pi = 1$ $\quad = 1/4 \left[\cos 2x \right]_0^{2\pi}$

$$1/4 \left[\cos 4\pi - \cos 0 \right]$$

$$-1/4 \; 1$$

⇒ Orthogonal wave function

*** For Example**

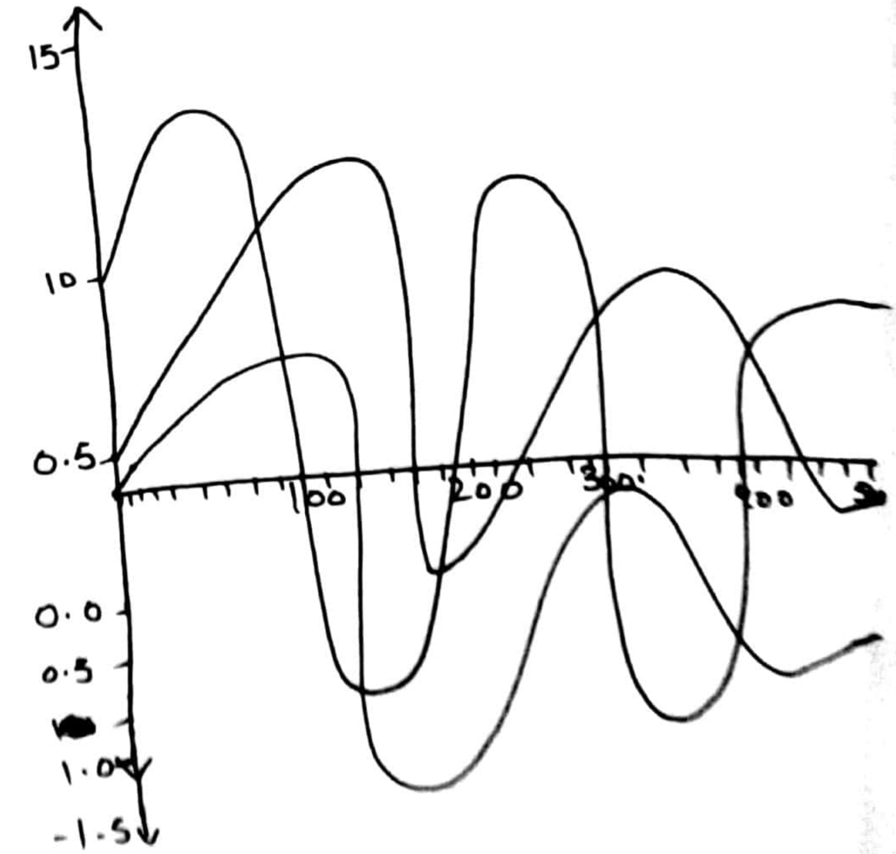
(2)

$$\int \psi_i^* \psi_j \, d\tau = 0$$

Both **sinx** and sin2x are eigin function of d/dx Show if **sinx** and sin2x are orthogonal.

$$\int \sin ax \sin bx \, dx = \frac{\sin(a-b)x}{2(a-b)} - \frac{\sin(a+b)x}{2(a-b)} + c$$

$$\int_0^{2\pi} \sin x \sin 2x \, dx = \frac{\sin(1-2)x}{2(1-2)} - \frac{\sin(1+2)x}{2(1-2)} + c = 0$$



Expection value.

$$\langle x \rangle = \int \psi_i^* \, X \, \psi_j \, d\tau$$

* Calculate the average value of the distance of e- from the h of H-atom

$$\Psi_{H-e} = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0}$$

$$\langle r\rangle = \int \Psi_i^* r \Psi_j \, d\tau = \frac{1}{\pi a_0^3} \int_0^\infty r^3 e^{-2r/a_0}$$

$$\langle r\rangle = \int \Psi_i^* r \Psi_j \, d\tau = \frac{1}{\pi a_0^3} \int_0^\infty r^3 e^{-2r/a_0} dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi$$

$$\int_0^\infty x^n e^{-ax} dx = \frac{n!}{n+1}$$

$$\frac{1}{\pi a_0^3} \frac{3! a_0^4}{2^4} \times 2 \times 2\pi = \frac{3}{2} a_0 = 79.4 \text{ Pm}$$

⇒Uncertainty Principle:-

Uncertainty in position along an axis

uncertainty in leaner momentum

$$\Delta p \Delta q \geq \frac{1}{2} \hbar$$

uncertainty the calculate the minimum uncertainty in the position of mass 1.0g and the speed is known with 1ums^{-1}

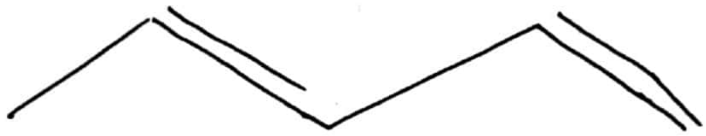
$$\Delta q \geq \frac{\hbar}{2\Delta p} = \frac{\hbar}{2m\Delta v}$$

$$\geq \frac{1.055 \times 10^{-34} Js}{2(1.0 \times 10^{-3} kg)(1 \times 10^{-6} ms^{-1})}$$

$$\geq 5 \times 10^{-26} m$$

Probability (particle in box)

Wave function of conjugated electron of Polyene can be appoximated by PAB. Find probability of locating electron between $X = 0$ and $X = 0.2nm$ in the lowest state in conjugated molecule of lenght 1.0m



$$\int_0^l \Psi_n \, dx = \frac{2}{L}\int_0^l \sin^2 \frac{n\pi x}{L} \, dx$$

$$= l/L - \frac{1}{2n\pi} \sin \frac{2\pi n l}{L}$$

$0.05 =$ when $n = 1$ $L = 1.0$ and $l = 0.2nm$

Scanned with CamScanner

⇒Normalization of the wave function

Normalization is the scalling of wave functions So that all the probability add to 1.. A normalized Wave function would be said to be normalized if it is not 1 and is instead equal to Some other Constant we incorporate That Constant into the wave function to normalize.

$$\int_0^a \Psi_2 \, dx = 1$$

Putting the value of ψ_2.

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

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

Since, $\sin^2\theta = \left(\frac{1 - \cos 2\theta}{2}\right)$

where, $\theta = \left(\frac{n\pi x}{a}\right)$

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

$\psi^*(x)\,\psi(x)$

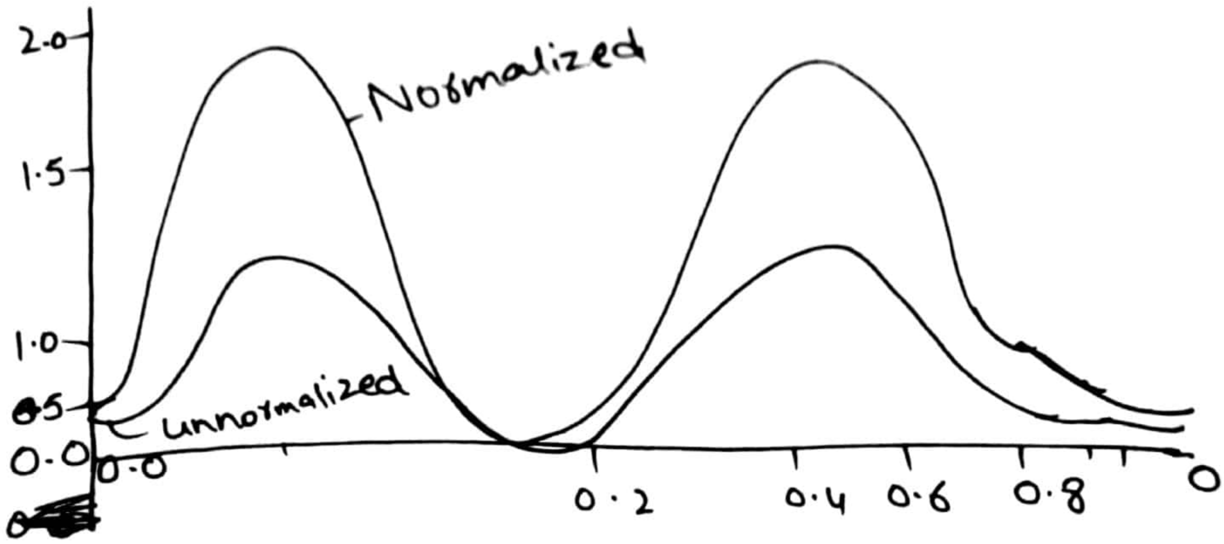
$$\int_{-\infty}^{\infty} \psi^*(x)\,\psi(x)\,dx = 1$$

⇒ Example:-

n = 2 State for a particle in a box of lenght L = 1

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

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



* Unnormalized - probability sum to 0.5 un-Physical.
* Normalized - probability sum to 1.0 Physical

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

$\frac{1}{2} A^2$ is constant is taken out side the integration sign.

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

Putting the value of limits,

$$\frac{A^2}{2}\left[a - \frac{a}{2n\pi}\,, \sin 2n\pi\right] = 1$$

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

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

The experssion for Eigen function is

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

Similiarly probability for folding a particle foo a particular of "x" is given by Taking the square ψ:

$$\psi^2 = \frac{2}{a} \cdot \sin^2 \cdot \left(\frac{n\pi x}{a}\right)$$

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

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

$$\frac{1}{2\pi}(\pi) = \frac{1}{2} \text{ Not normalized}$$

=>Example:-

Normalize a wave function for a particle in a box of lenght L given by.

$$\psi(x) = x(L-X)$$

$$\int \psi^*(x)\psi(x)\,dx = \int_0^L [Ar[L-x)][Ar(L-x)]dx$$

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

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

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

$$\frac{A^2 L^2}{30} = 1 \text{ if normalized}$$

$$\Rightarrow A \frac{\sqrt{30}}{L5} = \psi(x) = \frac{\sqrt{30}}{L5x}(L-x)$$

our final normalized wave function