Wave-function:-

for De-Broglie waves or matter waves associated with a moving particle, the quantity that vary with space and time is called wave function of the particle.

The temporal and spatial evolution of a quantum mechanical particle is described by a wave function $\psi(x,t)$ for 1-D motion and $\psi(\vec{r},t)$ for 3-D motion. It contains all possible information about the state of the system.

Conditions for a physically accepted, well behaved, realistic wave function:-

(i) $\psi(x,t)$ should be finite, single-valued and continuous everywhere in space.

(ii) $\frac{d\psi}{dx}$ should be continuous everywhere in space.

But $\frac{d\psi}{dx}$ may be discontinuous in some cases as follows:

(a) If the potential under which the particle is moving has an infinite

Numerical

1. Which of the following wave function is acceptable as the Solution of Schrodinger equation for all values of x?

(a) $\psi(x) = A\sec x$

(b) $\psi(x) = A\tan x$

(c) $\psi(x) = Ae^{x^2}$

(d) $\psi(x) = Ae^{-x^2}$

Sol $\psi(x) = A\sec x$ and $\psi(x) = A\tan x$

is not finite at $x = \frac{\pi}{2}$

$\psi(x) = Ae^{x^2}$ is not finite at $x = \pm\infty$

$\psi(x) = Ae^{-x^2}$

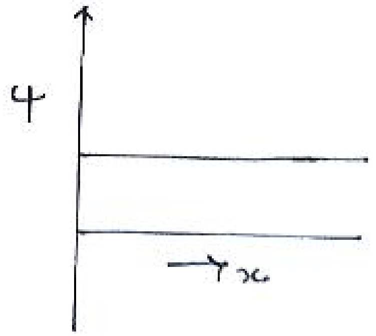
is finite everywhere in Space $\pm\infty$

$e^{-\infty} = 0$

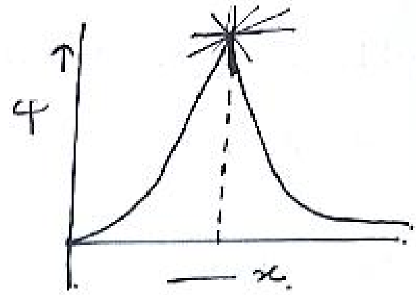
Correct option is (d)

2.) Which of the following wave-function cannot have physical Significance

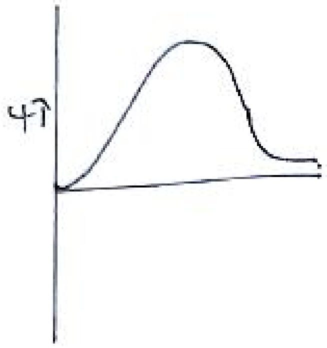
(a)



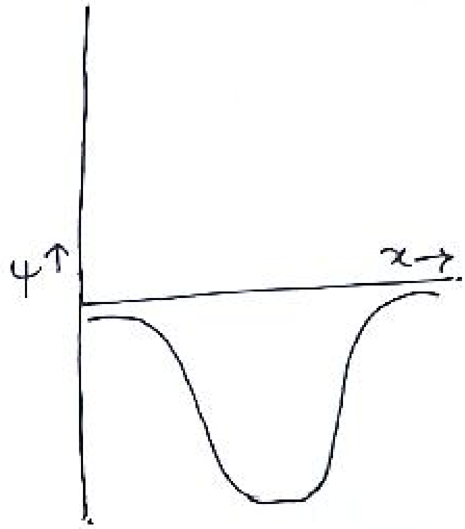
(e)



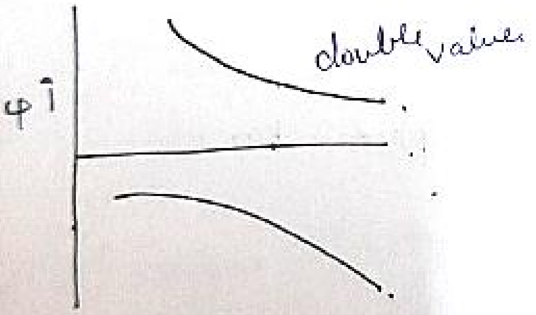
(b)



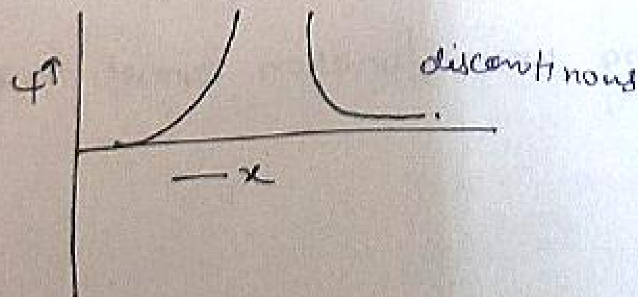
(f)



(c)

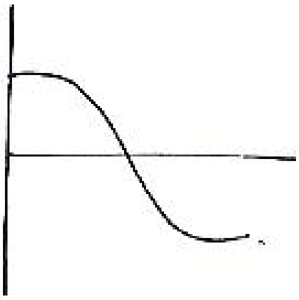


(d)

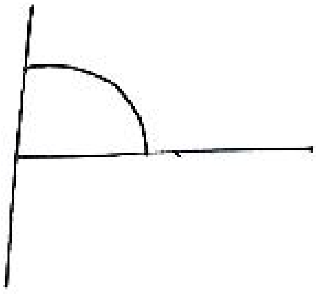


Sol:- a, b, and f have physical Significance.

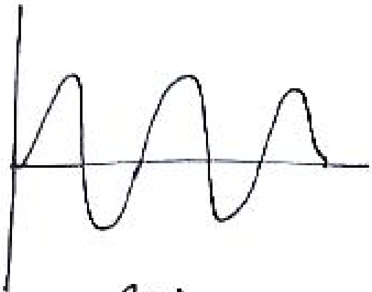
3.)



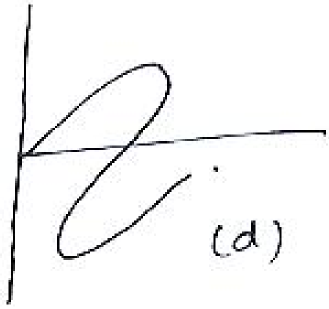
(a)



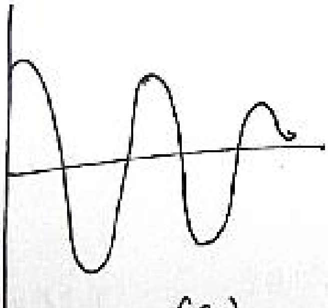
(b)



(c)



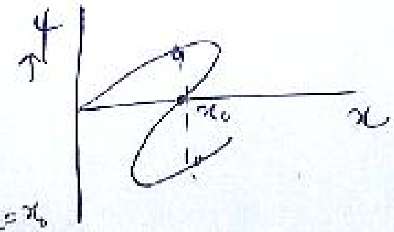
(d)



(e)

(a) finite, single valued, continous.

Acceptable wave function (a), (b), (c)



(d) Not acceptable

Multiple value at $x=x_0$

(c) $\psi(x) =$ finite, Single value, continous

$\frac{d\psi}{dx} =$ amplitude is lies in this case.

If amplitude is not decreasing then it is cos type curve so there is some decreasing function is multiplied with cos function or $e^{-\lambda x} \cos x$.

$\frac{d\psi}{dx} =$ continous

at every point tangent is one.

$\int_{-\infty}^{+\infty} \psi^* \psi \, dx =$ finite

Physical significance

Only (d) wave function is not acceptable.

Among the following wave function which represent the physically acceptable wave function.

(i) $3\sin\pi x$ (2) $4-|x|$

(iii) $\pm\sqrt{5x}$ (4) $e^{-\lambda x}$

Note $e^{-\infty} = 0$

(i) $3\sin\pi x$.

for $x = +\infty$ or $-\infty$.

$\sin\theta = -1$ to 1.

ψ. finite. for single value of θ.

ψ will be single valued continous.

(2) $\frac{d\psi}{dx} = 3\pi\cos\pi x$

at $x = \pm\infty$ $\cos\theta = -1$ to 1.

$\frac{d\psi}{dx} =$ finite.

Square integral:- $\int_{-\infty}^{+\infty} \psi^{*}\psi \, dx =$ finite

$$\int_{-\infty}^{+\infty} 3\sin\pi x \; 3\sin\pi x \, dx$$

$$= 9\int_{-\infty}^{+\infty} \sin^2\pi x \, dx$$

$$9 \int_{-\infty}^{+\infty} \left[\frac{1 - \cos 2\pi x}{2}\right] dx$$

$$9 \underbrace{\int_{-\infty}^{+\infty} \frac{1}{2} dx} - \frac{1}{2}\int_{-\infty}^{+\infty} \cos 2\pi x \, dx.$$

$$\underbrace{\frac{9}{2}\left[x\right]_{-\infty}^{+\infty}}_{\infty} - \frac{1}{2}\int_{-\infty}^{+\infty} \cos 2\pi x \, dx$$

So This wave is not acceptable.

(2) $f = \pm\sqrt{5x}$

It is not finite, for $x = \infty$ $f = \infty$.

for single value of x,

f gives double value

Suppose $x = 2$

$f = +\sqrt{10}, -\sqrt{10}$

Square integral $\int_{-\infty}^{+\infty} \psi^* \psi \, d\tau$

$$\int_{-\infty}^{+\infty} \sqrt{5x} \cdot \sqrt{5x} \, dx$$

$$\int_{-\infty}^{+\infty} 5x \, dx$$

$$= \underbrace{5\int_{-\infty}^{+\infty} x \, dx}_{\infty}$$

$$=$$

This wave funct is acceptable..

$f = 4 - |x|$

$x = \infty$, $f = \infty$

for $x \rightarrow$ single valued, ; f is single value.

At = $x = 0$, f is finite.

$x = 0$, $f = 4$.

Continous

$\frac{df}{dx} = -1$ for +ve side $f = 4 - x$.

for -ve side $f = 4 + x$

$\frac{df}{dx} = 1$.

At $x = 0$, function is single valued but its derivative has ∞ no of value

$\frac{df}{dx}$ is discontinuous $\left\{ \begin{array}{l} \text{This wave function} \\ \text{is not acceptable?} \end{array} \right.$

Which of the following wave function represent acceptable wave function of the particle in the range $-\infty \leq x \leq \infty$

(a) $\phi(x) = A \tan x$, $A > 0$

(b) $\phi(x) = B \cos x$, $B =$ real

(c) $\phi(x) = c \exp\left(\frac{-D}{x^2}\right)$, $C > 0$, $D < 0$

(d) $\phi(x) = Exe^{-Fx^2}$, $E, F > 0$

(a) $\phi(x) = A\tan x$

$x = \pm\infty$

$\phi(x) = \frac{\sin\theta}{\cos\theta} = \frac{\sin\infty}{\cos\infty}$ = Not finite.

$x = \frac{\pi}{2}$, $\phi(x) = \infty$

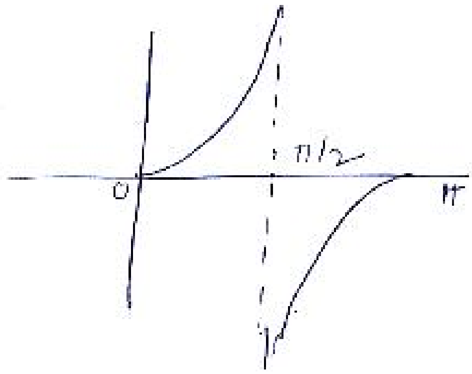
for single value of x, $\phi(x)$ is single valued.

Continous

At $\frac{\pi}{2}$, continous.

break

So At $x = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}$



$\phi(x)$ is discontinous

Not acceptable

(b) $\phi(x) = B\cos x$

for $x = -\infty$ to $+\infty$, $\phi(x) \rightarrow$ finite

Single valued

$\phi(x) = B\cos x$

It is continous

$\frac{d\phi}{dx} = -B\sin x$

Square integral $= |B|^2 \int_{-\infty}^{+\infty} \cos^2 x \, dx = \infty$

Not acceptable

(3) $\phi(x) = C \exp\left(\frac{-D}{x^2}\right)$

$x = 0$, $\phi(x) = \infty$

in all space

$\phi(x) = C \exp\left(\frac{-D}{x^2}\right)$

becoz $D < 0$

Not acceptable

(4) $\phi(x) = Exe^{-Fx^2}$.

This is the product of two function's ψ_1 and ψ_2.

$\psi_1 = x$, $\psi_2 = Ee^{-Fx^2}$

At $x = \pm\infty$, $\psi_1 = \pm\infty$, $\psi_2 = 0$

But for the product

$x = 0$

$\phi(x) = 0 \times 1 = 0$

$x \uparrow$, $\psi_1 \uparrow$ and $\psi_2 \downarrow$

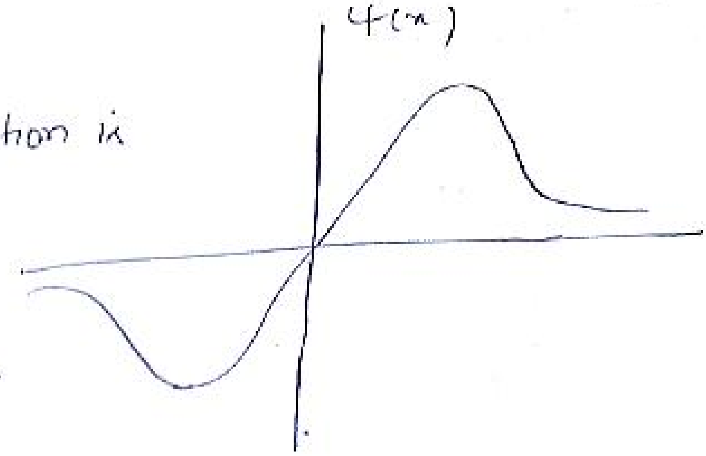
$\psi_1 \rightarrow$ increasing function

$\psi_2 \rightarrow$ decreasing function.

Slope of ψ_2 is larger than ψ_1 (Slope of ψ_1 is Constant)

So total product dies

$\psi = \psi_1 \psi_2$



The slope of decreasing function is large

So Total slope tends to 0.

for $x = -1$

$\psi_1 = +x$

$\psi_2 = Ee^{-\beta x^2} = Ee^{-\beta(-1)^2}$

ψ_1 and ψ_2 both are decreasing functions.

So product is Incs. upto some value and then it starts ↑) tend to zero

* If there is addition of two function then

$\psi = \psi_1 + \psi_2$.

ψ_1 and ψ_2 are continous then ψ will be continous

Same condition for derivative.

ψ is continous and $\frac{d\psi}{dx}$ is also continous

Square Integrable:- $\int_{-\infty}^{+\infty} \psi^* \psi \, dx$

$|E|^2 \int_{-\infty}^{+\infty} x^2 e^{-2\beta x^2} dx$.

$2E^2 \int_0^{\infty} x^2 e^{-2\beta x^2} dx$

$=$ finite

Acceptable

ψ Should be normalized

$$\int_{-\infty}^{+\infty} |\psi|^2 d\tau = 1 \quad = \int_{-\infty}^{+\infty} \psi^* \psi \, d\tau = 1.$$

Meaning of normalized

at $-\infty$ to ∞ within the given range particle will present

A particle of mass m is confined in the 1-D box extending from $-2L$ to $2L$. The wave function of the particle in this state.

$$\psi(x) = \psi_0 \cos\left(\frac{\pi x}{4L}\right)$$

Where ψ_0 is constant.

$$\int_{-\infty}^{+\infty} \psi^* \psi \, d\tau = 1$$

$$\int_{-2L}^{+2L} |\psi|^2 \cos^2\left(\frac{\pi x}{4L}\right) dx = 1.$$

$$|\psi|^2 \int_{-2L}^{+2L} \frac{1}{2} \left(1 + \cos\frac{2\pi x}{4L}\right) dx = 1$$

$$\frac{1}{2} \cdot |\psi|^2 \left[x - \sin\left(\frac{2\pi x}{4L}\right) \times \frac{4L}{2\pi} \right]_{2L}^{+2L} = 1.$$

$$\frac{1}{2}|\psi_0|^2\left[2L - \frac{4L}{2\pi}\sin\left(\frac{2\pi}{4L}\cdot 2L\right) + 2L + \frac{4L}{2\pi}\sin\left(\frac{2\pi}{4L}\cdot 2L\right)\right]^{12} = 1$$

$$\frac{1}{2}\left[4L - 0\right]|\psi_0|^2 = 1.$$

$$|\psi_0|^2 = \frac{2}{4L}$$

$$= \frac{1}{2L}$$

$$\boxed{|\psi_0| = \sqrt{\frac{1}{2L}}}$$

\# $\psi = N x \exp\left(\frac{-x^2}{2}\right)$ Calculate the normalization constant

$$= \int_{-\infty}^{+\infty} \psi^* \psi \, d\tau = 1$$

$$= \int_{-\infty}^{+\infty} N x \exp\left(\frac{-x^2}{2}\right) \cdot N x \exp\left(\frac{-x^2}{2}\right) dx = 1$$

$$N^2 \int_{-\infty}^{+\infty} x^2 \exp(-x^2)\, dx = 1$$

$$N^2 \int_{-\infty}^{+\infty} x^2 e^{-x^2} dx = 1$$

$$N^2 \cdot \frac{\sqrt{\pi}}{2} = 1$$

$$\boxed{N = \left(\frac{2}{\sqrt{\pi}}\right)^{1/2}}$$

$$\psi = \left(\frac{2}{\sqrt{\pi}}\right)^{1/2} x \exp\left(\frac{-x^2}{2}\right)$$

$$\left(\frac{-x^2}{2}\right)$$

$\psi(x) = A\exp\left(\frac{-x^2}{a^2}\right)\exp(ikx)$

$\Downarrow$

find normalization constant

$$\int_{-\infty}^{+\infty} \psi^* \psi \, d\tau = 1$$

$$\int_{-\infty}^{+\infty} A\exp\left(\frac{-x^2}{a^2}\right)\exp(ikx) \cdot A\exp\left(\frac{-x^2}{a^2}\right)\exp(-ikx)\,dx = 1$$

$$A^2 \int_{-\infty}^{+\infty} \exp\left(-\frac{2x^2}{a^2}\right) dx = 1$$

$$A^2 \left(\frac{\pi}{2/a^2}\right)^{1/2} = 1$$

$$A = \sqrt{\frac{2}{\pi}}\, a.$$

Expectation Value:-

for a dynamical variable expectation value

$$\langle A \rangle = \frac{\int_{\text{all sp}} \psi^* A \psi \, dx}{\int_{\text{all space}} \psi^* \psi \, dx}$$

The expectation value of P^2 in this state is $\psi = \sqrt{\frac{1}{2L}} \cos\left(\frac{\pi x}{4L}\right)$ 4.

(a) 0 (b) $\frac{\hbar^2\pi^2}{32L^2}$ (c) $\frac{\hbar^2\pi^2}{16L^2}$ (D) $\frac{\hbar^2\pi^2}{8L^2}$

range $-2L$ to $2L$

$$P = \frac{-\hbar^2 d^2}{dx^2}$$

$$\langle p^2 \rangle = \int_{-2L}^{+2L} \left(\sqrt{\frac{1}{2L}} \cos\left(\frac{\pi x}{4L}\right)\right)\left(-\hbar^2 \frac{d^2}{dx^2}\right)\left[\sqrt{\frac{1}{2L}} \cos\left(\frac{\pi x}{4L}\right)\right] dx$$

$$= -\hbar^2 \cdot \frac{1}{2L} \int_{-2L}^{+2L} \cos\frac{\pi x}{4L} \frac{d^2}{dx^2}\left[\cos\left(\frac{\pi x}{4L}\right)\right] dx$$

$$\frac{d^2}{dx^2}\left(\cos\frac{\pi x}{4L}\right) = \cos\frac{\pi x}{4L} \times \left(\frac{\pi}{4L}\right)^2$$

$$\frac{d}{dx}\left(\cos\frac{\pi x}{4L}\right) = -\sin\left(\frac{\pi x}{4L}\right) \cdot \left(\frac{\pi}{4L}\right)$$

$$\frac{d}{dx}\left(-\sin\left(\frac{\pi x}{4L}\right) \cdot \left(\frac{\pi}{4L}\right)\right) = \cos\left(\frac{\pi x}{4L}\right) \cdot \left(\frac{\pi}{4L}\right)^2$$

$$= +\hbar^2 \cdot \frac{1}{2L} \int_{-2L}^{+2L} \cos\left(\frac{\pi x}{4L}\right) \cos\left(\frac{\pi x}{4L}\right) \cdot \left(\frac{\pi}{4L}\right)^2 dx$$

$$= \hbar^2 \cdot \frac{1}{2L} \cdot \left(\frac{\pi}{4L}\right)^2 \int_{-2L}^{+2L} \cos^2\left(\frac{\pi x}{4L}\right) dx$$

$$= \frac{\hbar^2}{2L}\left(\frac{\pi}{4L}\right)^2 \cdot \cancel{2}\int_0^{2L} \frac{1+\cos\frac{2\pi x}{4L}}{\cancel{2}}\, dx$$

$$= \frac{\hbar^2}{2L}\left(\frac{\pi}{4L}\right)^2 \left[2L + \frac{2L}{\pi}\sin\frac{\pi}{2L}\times 2L\right]$$

$$= \frac{\hbar^2\pi^2}{16L^2}.$$

\# Calculate the expectation value of P and P^2. for wave function?

$$\psi(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right) \quad , \; 0<x<L$$

$$= 0 \qquad \text{otherwise.}$$

$$\langle p\rangle = \int_0^L \psi^*(x)\left(-i\hbar\frac{d}{dx}\right)\psi(x)\, dx$$

Wave is already Normalized $\int_{-\infty}^{\infty} \psi^*\psi = 1$

$$= \int_0^L \sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}\left(-i\hbar\frac{d}{dx}\right)\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}\, dx$$

$$= \frac{2}{L}\int_0^L \sin\frac{\pi x}{L}\left(-i\hbar\frac{d}{dx}\right)\sin\frac{\pi x}{L}\, dx$$

$$= \frac{2}{L}\int_0^L \sin\frac{\pi x}{L}(-i\hbar)\cos\left(\frac{\pi x}{L}\right)\times\frac{\pi}{L}\, dx$$

$$= \frac{2}{L}\times(-i\hbar)\times\frac{\pi}{L}\int_0^L \frac{1}{2}\sin\frac{2\pi x}{L}\, dx$$

$$= \frac{\pi}{L^2}(-i\hbar)\left[\cos\frac{2\pi x}{L}\right]_0^L \cdot \left(\frac{L}{2\pi}\right)$$

$$= -\frac{i\hbar}{2L}\left[\cos 2\pi - \cos 0^\circ\right]$$

$$= -\frac{i\hbar}{2L}(1-1) = 0$$

$$\langle p^2\rangle = \int_0^L \psi^*\left(-\hbar^2 \frac{d^2}{dx^2}\right)\psi\, dx$$

$$= -\hbar^2 \int_0^L \frac{2}{L}\sin\frac{\pi x}{L}\frac{d}{dx}\left[-\cos\frac{\pi x}{L}\right)\times\left(\frac{\pi}{L}\right)dx.$$

$$= \hbar^2 \cdot \frac{2}{L}\int_0^L \sin\frac{\pi x}{L}\sin\left(\frac{\pi x}{L}\right)\times\left(\frac{\pi}{L}\right)^2 dx.$$

$$= \frac{2\hbar^2}{L}\left(\frac{\pi}{L}\right)^2\int_0^L \sin^2\frac{\pi x}{L}\, dx$$

$$= \frac{2\pi^2\hbar^2}{L^3}\int_0^L \left(\frac{1-\cos\frac{2\pi x}{L}}{2}\right)dx$$

$$= \frac{2\pi^2\hbar^2}{L^3 \cdot 2}\left[x - \frac{\sin\frac{2\pi x}{L}}{\frac{2\pi}{L}}\right]_0^L.$$

$$= \frac{\pi^2\hbar^2}{L^3}\left[L - \frac{\sin 2\pi}{2\pi/L} - 0 + 0\right]$$

$$\boxed{\langle p^2\rangle = \frac{\pi^2\hbar^2}{L^2}}$$

\# find the expectation value of position and momentum of a particle whose wave-function is

$$\psi(x) = e^{-x^2/a^2 + ikx} \quad \text{in all space.}$$

Calculate $\langle P \rangle$ and $\langle x \rangle$

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} \psi^* x \psi \, dx}{\int_{-\infty}^{+\infty} \psi^* \psi \, dx}$$

$$\langle x \rangle = \int_{-\infty}^{+\infty} \psi^* x \psi \, dx$$

$$= \int_{-\infty}^{+\infty} e^{-x^2/a^2 - ikx} \cdot x \cdot e^{-\frac{x^2}{a^2} + ikx} \, dx$$

$$= \int_{-\infty}^{+\infty} \underbrace{x}_{\text{odd}} \cdot \underbrace{e^{-2x^2/a^2}}_{\text{even}} \, dx$$

$$= 0$$

this wave function is odd integral will be zero

$$\langle p \rangle = \frac{\int_{-\infty}^{+\infty} e^{-\frac{x^2}{a^2} - ikx} \left(-i\hbar \frac{d}{dx}\right) e^{-\frac{x^2}{a^2} + ikx} \, dx}{\int_{-\infty}^{+\infty} e^{-\frac{x^2}{a^2} - ikx} \cdot e^{-\frac{x^2}{a^2} + ikx} \, dx}$$

$$= \frac{-i\hbar \int_{-\infty}^{+\infty} e^{-\frac{x^2}{a^2} - ikx} e^{-\frac{x^2}{a^2} + ikx} \left(\frac{-2x}{a} + ik\right) dx}{2 \int_{0}^{\infty} e^{-2x^2/a^2} \cdot x \, dx}$$

$$= \frac{-i\hbar \int_{-\infty}^{+\infty} e^{-\frac{2x^2}{a^2}} \left(\underbrace{-\frac{2x}{a}}_{odd} + ik\right) dx}{2\int_0^{\infty} e^{-2x^2/a^2} dx}$$

$$= \frac{-i\hbar\, 2\int_0^{\infty} e^{-2x^2/a^2}\, ik\, dx + \overbrace{e^{-2x^2/a^2}\left(-\frac{2x}{a}\right)}^{0}}{2\int_0^{\infty} e^{-2x^2/a^2} dx}$$

$$= \frac{\hbar k \int_0^{\infty} e^{-2x^2/a^2} dx}{\int_0^{\infty} e^{-2x^2/a^2} dx}$$

$$\boxed{= \hbar k}$$

Eigen value and Eigen function:

For every observable quantity, there is a linear operator. Let $\psi(x)$ be a well-behaved function in a given system. Now, if this is operated on by the operator $\hat{A}$ such that it satisfies the equation given below

$$\hat{A}\psi(x) = a\psi(x) \quad \text{--- (A)}$$

Where a is eigen value

The wave function that satisfies the eq (A) or the operator $\psi(x)$ is known as eigen functions and corresponding observable quantity (a) is called eigen value and the eq (A) is called eigen value eq. for $\psi = e^{ax}$ $\quad \hat{A} = \frac{d}{dx}$.

<u>Operators:-</u>

If $D_x = \frac{i\, d}{\partial x}$ and $D_x^2 = -\frac{\partial^2}{\partial x^2}$ and for both cases $\psi(x) = \sin kx$

$\psi(x) = \sin kx$

find D_x and D_x^2 are only operator.

$$D_x = \frac{i\, d}{\partial x}$$

$$= i \frac{\partial}{\partial x} \psi$$

$$= i \frac{\partial}{\partial x} (\sin kx) = i \cos kx \times k$$

$$D_x^2 = -\frac{\partial^2}{\partial x^2} \psi$$

$$= -\frac{\partial^2}{\partial x^2} (\sin kx)$$

$$= \sin kx\, k^2$$

$$= k^2 \psi(x)$$

The operator $\left(x + \frac{d}{dx}\right)$ has the eigen value α. Determine the corresponding wave function.

Eigen value equation $\left(x + \frac{\partial}{dx}\right)\psi = \alpha\psi$

$$\frac{d\psi}{dx} = \alpha\psi - x\psi$$

$$\frac{d\psi}{dx} = (\alpha - x)\psi$$

$$\int \frac{d\psi}{\psi} = \int (\alpha - x)dx$$

$$\ln \psi = \left(\alpha x - \frac{x^2}{2}\right) + \ln \psi_0$$

$$\psi = \psi_0 \exp\left(\alpha x - \frac{x^2}{2}\right)$$

find the constant B which makes $e^{-\alpha x^2}$ an eigen function of the operator $\left(\frac{d^2}{dx^2} - Bx^2\right)$ What is the corresponding eigen values?

$$\left(\frac{d^2}{dx^2} - Bx^2\right)e^{-\alpha x^2} = \left(4a^2x^2 - 2a + Bx^2\right)e^{-\alpha x^2}$$

for e^{-ax^2} to be eigen function of the operator $\left(\frac{d^2}{dx^2} - Bx^2\right)$ then the eigen

$(4a^2x^2 - 2a - Bx^2)$ must be independent of x i.e

$$(4a^2 - B) = 0$$

$$B = 4a^2.$$

$$\left(\frac{d^2}{dx^2} - Bx^2\right)e^{-\alpha x^2} = -2ae^{-\alpha x^2}.$$

eigen value of the operator is $(-2a)$