1) Schrödinger's equation

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$= \frac{\partial^2}{\partial x^2} \ (1D)$$

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

Hamiltonian ← → wave fn.

- single valued and cont.
- $\frac{\partial \psi}{\partial x}$ cont. and single valued
- ψ must be normalizable

$$\int_{\text{all space}} \psi^* \psi \underbrace{d\tau}_{\text{volume}} = 1$$

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

2) Operators : operate on wavefn. of quantum particle to give you a <u>measurable</u> quantity

energy, K.E, position, momentum, P.E.

HOW?

using operator and wavefn.

suppose you have a wfn and you need to know the K.E., P.E., position, P.E. of that particle how will you proceed?

<u>Q1.</u> Find momentum of $\psi(x) = Ae^{-x^2/a^2}$

<u>2.</u> find ~~a~~ energy of free particle with wavefn. $\psi(x) = Ae^{ikx}$

<u>1.</u> $$\langle p_x \rangle = \int_{-\infty}^{\infty} \psi^* p_x \psi \, dx$$

$$= \int_{-\infty}^{\infty} Ae^{-x^2/a^2} \left(-i\hbar \frac{d}{dx} Ae^{-x^2/a^2}\right) dx$$

$$= 0$$

Sol 2. $\langle E \rangle = \int_{-\infty}^{\infty} \psi^* H \psi \, dx$

$$= \int_{-\infty}^{\infty} Ae^{-ikx} \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} Ae^{ikx} \, dx$$

$$= \frac{-A^2 (ik)^2 \hbar^2}{2m} \int_{-\infty}^{\infty} e^{-ikx} \cdot e^{ikx} \, dx$$

$$\cancel{= \frac{+A^2 \hbar^2 k^2}{2m} \int_{-\infty}^{\infty} e^{k^2 x^2} \, dx}$$

$$= \frac{A^2 \hbar^2 k^2}{2m} \int_{-\infty}^{\infty} e^{-ikx} \cdot e^{ikx} \, dx$$

3) now, eigenfunction and eigen value.

$$\hat{A} \psi = a \psi$$

eigenfn. eigen value (constant +)

now questions

1) $\hat{A} = \text{K.E.} = \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \qquad \psi = Ae^{-\frac{x^2}{a^2}}$

$$\hat{A} \psi = \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \left(Ae^{-\frac{x^2}{a^2}} \right)$$

$$= \frac{A\hbar^2}{ma^2} \left(1 - \frac{2x^2}{a^2} \right) e^{-x^2/a^2}$$

$$= \frac{A\hbar^2}{ma^2} \psi(x) - \frac{2A\hbar^2}{ma^4} x^2 \psi(x)$$

$$\hat{A} \psi \neq a \psi$$

2) $\hat{A} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$ $\quad \psi(x) = Ae^{ikx}$

$$\hat{A}\psi = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} Ae^{ikx}$$

$$= -\frac{\hbar^2}{2m}(ik)^2 Ae^{ikx}$$

$$= \frac{\hbar^2 k^2}{2m} Ae^{ikx} = a\psi$$

now $\psi(x)$ here is an eigenfn.

$a = \frac{\hbar^2 k^2}{2m}$ is eigenvalue corr. to given $\psi(x)$.

<u>Ques.</u> Is the function $Ae^{-x/a}$ an eigenfn. of KE operator of a particle? NO

4th Concept   Operator : Properties

1) Linear   a) $A[f(x) + g(x)] = Af(x) + A g(x)$

b) $A[c f(x)] = c A f(x)$

Consider $f(x) = \sin x$ $g(x) = \cos x$ $A = \frac{d}{dx}$

LHS a) $\frac{d}{dx}(\sin x + \cos x) = \frac{d}{dx}\sin x + \frac{d}{dx}\cos x$

b) $\frac{d}{dx}[c \sin x] \overset{LHS}{=} 0 . \sin x + c \frac{d}{dx}\sin x = c \cos x$

RHS $c \frac{d}{dx}\sin x = c \cos x$ LHS = RHS

So $\frac{d}{dx}$ is a linear operator.

2) Commutative $[A, B] = AB - BA = 0$

$A = x$ $B = p_x$, $f(x) = \sin x$

$x \, p_x \sin x - p_x \, x \sin x$

$x\left(-i\hbar\frac{d}{dx}\right)\sin x + i\hbar\frac{d}{dx}(x \sin x)$

$-x i\hbar \cos x + x i\hbar \cos x + i\hbar \sin x$

$i\hbar \sin x$

$[x, p_x] = i\hbar$