B. Sc. (Semester -6)
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Unit : 3 – General Formalism of Wave Mechanics

THE ADJOINT OF AN OPERATOR AND SELF-ADJOINTNESS

Let us consider the integral

$$\int \phi^* A \psi d\tau \equiv (\phi, A\psi) \tag{1}$$

which involves two different functions ϕ and ψ and reduces to in the special case when $\phi = \psi$. It can be shown that one can always find another operator, called the *adjoint* of A and denoted by $A^\dagger$ (read A dagger), such that

$$\int \phi^* A\psi \, d\tau = \int (A^\dagger \phi)^* \psi \, d\tau, \quad \text{or} \quad (\phi, A\psi) = (A^\dagger \phi, \psi) \tag{2}$$

In other words, as far as the value of the integral is concerned, it makes no difference whether A acts on ψ or its adjoint $A^\dagger$ acts on the other wave function ϕ. Equation (2) serves to define the adjoint of any operator. From this definition it is easy to show

$$(A + B)^\dagger = A^\dagger + B^\dagger \tag{3}$$

and that if c is a complex number

$$(cA)^\dagger = c^* A^\dagger \tag{4}$$

i.e. in taking the adjoint, any complex number goes over into its complex conjugate. Further, since

$$\int \phi^* (A^\dagger \psi) \, d\tau = \left[\int (A^\dagger \psi)^* \phi \, d\tau\right]^* = \left[\int \psi^* A \phi \, d\tau\right]^* = \int (A\phi)^* \psi \, d\tau$$

we have

$$(A^\dagger)^\dagger = A \tag{5}$$

For the adjoint of the product of two operators A and B, by applying the definition given in Eq. (2) successively to A and B, one obtains

$$\int \phi^* AB\psi d\tau = \int (A^\dagger \phi)^* B\psi d\tau = \int (B^\dagger A^\dagger \phi)^* \psi d\tau,$$

or

$$(AB)^\dagger = B^\dagger A^\dagger \tag{6}$$

An operator A is said to be *self adjoint*[A] if its adjoint is equal to itself:

$$A^{\dagger} = A,$$

or

$$\int \phi^* A \psi \, d\tau = \int (A\phi)^* \psi \, d\tau, \quad \text{i.e., } (\phi, A\psi) = (A\phi, \psi) \tag{7}$$

Note that the product of two self-adjoint operators is *not* necessarily self-adjoint. For, if $A^{\dagger} = A$ and $B^{\dagger} = B$, then according to Eq. (4),

$$(AB)^{\dagger} = BA \tag{8}$$

Thus AB is self adjoint only if $BA = AB$, i.e., if A and B commute. However, the two combinations

$$(AB + BA) \quad \text{and} \quad i(AB - BA) \tag{9}$$

are both self-adjoint, as the reader may verify.

It is now a trivial matter to see that the expectation value of a self-adjoint operator is real, for on setting $\phi, = \psi$ in Eq. (7) it reduces to $\langle A \rangle = \langle A \rangle^*$. Thus self-adjoint operators are suitable for representing observable dynamical variables, and we proceed to study their most important properties. Incidentally, it may be observed that $A^{\dagger}A$ is always self-adjoint (even if A is not). Further, its expectation value is non-negative in *all* states. (Any operator with this property is said to be *positive*.)

$$\langle A^{\dagger}A \rangle = \int \psi^* A^{\dagger} A \, \psi \, d\tau = \int (A\psi)^* \, (A\psi) \, d\tau \geqslant 0 \tag{10}$$

since the integrand, heing the absolute square of the function $A\psi$, is nonnegative. Evidently if $\langle A^{\dagger}A \rangle$ is to vanish, the integrand must vanish identically. Thus,

$$\langle A^{\dagger}A \rangle = 0 \text{ implies } A\psi = 0 \tag{11}$$

* The eigenvalue problem; Degeneracy :-

For any operator A, the eigenvalue equation can be written as $A\phi_a = a\,\phi_a$ ----- (1)

If a function ϕ_a is such that the action of the operator A on it has the simple effect of multiplying it by a constant factor 'a', then ϕ_a is an eigenfunction of A belonging to the eigenvalue 'a'. The set of all eigenvalues of A is called the eigenvalue spectrum of A. The spectrum may be continuous, or discrete, or partly continuous and partly discrete.

If there exist only one eigenfunction corresponds to a given eigenvalue, then the eigenvalue is called non-degenerate.

If there are more than one eigenfunction for a given eigenvalue then it is called degenerate.

For any degenerate eigenvalue there is always an infinite numbers of eigenfunctions.

Now consider,

$$\left. \begin{aligned} A\phi_a &= a\phi_a \\ \text{and, } A\chi_a &= a\chi_a \end{aligned} \right\} \quad \text{--- (2)}$$

Multiplying above eqn by C_1 and C_2 respectively and adding we get

$$A(C_1\phi_a + C_2\chi_a) = a(C_1\phi_a + C_2\chi_a) \quad \text{--- (3)}$$

Hence $(C_1\phi_a + C_2\chi_a)$ is set of eigenfunction corresponding to a given value of eigenvalue. This set forms a linear space. This space is called eigenspace belonging to the eigenvalue a of A.

In general $\phi_{a1}, \phi_{a2} \ldots \phi_{ar}$, the set of functions such that every eigenfunctions belonging to a can be expressed as a linear combination

$$C_1\phi_{a1} + C_2\phi_{a2} + \cdots + C_r\phi_{ar}, \quad \text{------ (4)}$$

where $C_1, C_2, \ldots C_r$ are the suitable coefficients. $\phi_{a1}, \phi_{a2}, \ldots \phi_{ar}$ form a set of basis functions which spans the linear space.

There is an infinite number of ways of choosing a basis. But the numbers r is characteristic of the space. Hence there is a definite number r of linearly independent. This number is called the degree of degeneracy of the eigenvalue. We say that the eigenvalue is r-fold degenerate.

* Eigenvalues and Eigenfunctions of Self-Adjoint Operators :

Adjoint : $\int \phi^* A \psi \, d\tau = \int \psi^* A^\dagger \phi \, d\tau$

If the adjoint of an operator is itself an operator is called self adjoint operator.

$$A = A^\dagger \qquad \text{—— (1')}$$

or

$$\int \phi^* A \psi \, d\tau = \int (A^\dagger \phi)^* \psi \, d\tau \qquad \text{—— (1'')}$$

or

$$(\phi, A\psi) = (A^\dagger \phi, \psi) \qquad \text{—— (1''')}$$

Let A be a self-adjoint operator, and ϕ_a, ϕ_a' be two eigenfunctions, then

$$A\phi_a = a\phi_a \,, \quad A\phi_a' = a'\phi_a' \qquad \text{—— (4)}$$

The self-adjointness condition is

$$\int \phi^* A \psi \, d\tau = \int (A\phi)^* \psi \, d\tau \qquad \text{---- (5)}$$

Substituting $\phi = \phi_a$ and $\psi = \phi_a'$ in eqn (5) we get

$$\int \phi_a^* A \phi_a' \, d\tau = \int (A\phi_a)^* \phi_a' \, d\tau \qquad \text{----- (6)}$$

We have eigen eqn. $A\phi_a = a\phi_a$

Now multiplying this eqn by ϕ_a^* and taking integral we get

$$\int \phi_a^* A \phi_a \, d\tau = a \int \phi_a^* \phi_a \, d\tau \quad \text{------} \quad (7)$$

similarly we have $A \phi_a^* = a^* \phi_a^*$

Againg multiplying on both the sides by ϕ_a and taking integral we get

$$\int \phi_a A \phi_a^* \, d\tau = a^* \int \phi_a \phi_a^* \, d\tau \quad \text{----} \quad (8)$$

But A is self adjoint hence from eqns (7) & (8) we can write

$$(a - a^*) \int \phi_a^* \phi_a \, d\tau = 0 \quad \text{----} \quad (9)$$

But $\int \phi_a^* \phi_a \, d\tau \neq 0$

$$\therefore \quad a = a^* \quad \text{----} \quad (10)$$

Thus, the eigenvalues of a self-adjoint operator are real.

Now, if $\int \phi_a^* \phi_a \, d\tau = 0$

$$\text{then} \quad a \neq a^* \quad \text{----} \quad (11)$$

Hence, any two eigenfunctions belonging to unequal eigenvalues of a self-adjoint operator are mutually orthogonal.

The operator may have both normalizable and non-normalizable eigenfunctions. Thus the norm of ϕ_a may be either 1 or ∞. Therefore we write

$$\int \phi_a^* \phi_a' \, d\tau = \delta(a, a') \quad \text{------} \quad (12)$$

where $\delta(a, a') = 0$ for $a \neq a'$

and, $\delta(a, a') = 1$ if ϕ_a is normalizable
$= \infty$ if " " not normalizable

$\delta(a, a')$ is known as Kronecker delta function.

$$\delta(a, a') = \delta_{aa'} \quad \text{-----} \quad (13)$$

For an infinite norm of eigenfunctions we write

$$\delta(a, a') = \delta(a - a') \quad \text{----} \quad (14)$$

where $\delta(a - a')$ is the Dirac delta function.

Eqn (13) applies if a belongs to the discrete part of the eigenvalue spectrum and,

Eqn (14) in the case of eigenvalues belonging to the continuum part of the spectrum.

* The Dirac Delta function:

The dirac delta function is a certain function for which it gives infinite value at a particular point and zero everywhere. If a function is a finite at a perticular single point and zero for the other ~~points~~ points then its integral or area under the curve will be zero.

Now,

$$\int_{-\infty}^{\infty} \delta(x - x')\, dx = 1 \quad \text{----} \quad (1)$$

$$\left.\begin{aligned} \delta(x - x') &= 0, \quad x \neq x' \\ &= \infty, \quad x = x' \end{aligned}\right\} \quad \text{—} \quad (2)$$

The dirac delta function is also defined through the equation

$$\int_a^b f(x)\, \delta(x - x')\, dx = f(x'), \quad a < x' < b \quad \text{---} \quad (3)$$

Here x is a continuous variable. According to the definition, whatever the function $f(x)$ may be, the delta function appearing in the integral picks out the value of $f(x)$ at the single point x', and the integral does not take account the behaviour of $f(x)$ anywhere else.

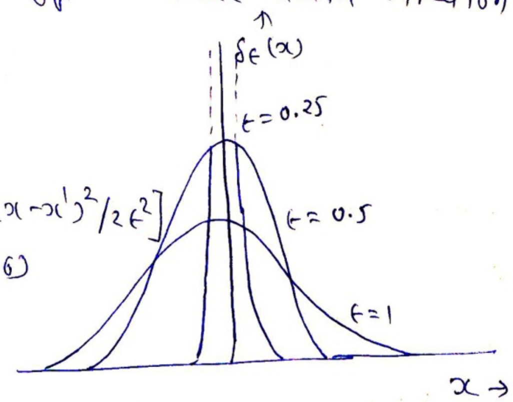
$$\therefore \quad \delta(x-x') = 0 \quad \text{for all } x \neq x' \quad --- (4)$$

At $x = x'$, the delta function cannot be finite at a single point and is zero everywhere. Its integral must vanish at a single point.

From eqn (3)

$$\delta(x, x') = \infty \quad \text{when } x = x' \quad ---- (5)$$

Figure shows the behaviour of dirac delta function $\delta_\epsilon(x-x')$ as $\epsilon \to 0$.



Here,

$$\delta_\epsilon(x-x') = (2\pi\epsilon^2)^{-1/2} \exp\left[-(x-x')^2/2\epsilon^2\right] \quad --- (6)$$

In the limit $\epsilon \to 0$ it satisfied eqn (5) and also the condition $\int \delta(x-x')\,dx = 1$ --- (7)

The three-dimensional Dirac delta function is defined by

$$\delta(\vec{x} - \vec{x}') = \delta(x-x')\,\delta(y-y')\,\delta(z-z') \quad --- (8)$$

* Observables : Completeness and Normalization of Eigenfunctions

If a dynamical variable is to be considered as observable, the operator representing ~~its~~ it must be self adjoint. A requirement is that, the eigenfunctions of the operator should be form of complete set. Any dynamical variable represented by a self-adjoint operator having a complete set of eigenfunctions qualifies to be called an observable.

Let A be a self adjoint operator of some physical problem. Its eigenfunctions $\{\phi_a\}$ are said to form a complete set if any arbitrary wave function ψ of the system can be 'expanded' into a linear combination

$$\psi = \sum C_a \phi_a + \int C_a \phi_a da \qquad \text{——— (1)}$$

The linear combination includes summation over the discrete part of the eigenvalue spectrum as well as integration over the continuous part. The assumption that a set $\{\phi_a\}$ is complete.

Let us evaluate the norm of ψ taken to be 1 in terms of the coefficients C_a. Now consider the case of an operator A whose eigenvalue spectrum is discrete, so that second term of eqn (1) will not be present. Using the orthonormality property of the ϕ_a,

$$\therefore \quad 1 = \int \psi^* \psi \, d\tau$$

$$= \int \Big[\sum_{a'} c_{a'}^* \phi_{a'}^* \Big] \Big[\sum_a c_a \phi_a \Big] d\tau$$

$$= \sum_{a'} \sum_a c_{a'}^* c_a \int \phi_{a'}^* \phi_a \, d\tau$$

$$= \sum_{a'} \sum_a c_{a'}^* c_a \, \delta(a', a)$$

$$= \sum_a c_a^* c_a \, \delta(a, a) \qquad \left[\because \text{ when } a = a' \text{ we get a single value} \right] \quad \text{--- (2)}$$

Now, there are two posibilities corresponding to $\delta(a,a) = 1$ or ∞.

But $\delta(a,a) = \infty$ must be rejected because it makes the eqn. (2) inconsistent.

Hence we conclude that "the eigenfunctions belonging to discrete eigenvalues are normalizable".

Setting $\delta(a,a') = \delta_{aa'}$ in above eqn., we obtain

$$\sum_a |c_a|^2 = 1 \qquad \text{------ (3)}$$

If we had a continuous instead of a discrete spectrum for a, integrals would appear in the place of summation in eqn (2), and it becomes

$$1 = \int c_a \, da \int c_{a'}^* \, \delta(a, a') \, da' \qquad \text{----- (4)}$$

The integral over a' vanishes if $\delta(a,a')$ is Kronecker delta and hence eqn (4) would be inconsistent. Hence we have to take $\delta(a,a')$ as the Dirac delta function.

Therefore, "the eigenfunctions belonging to continuous eigenvalues are of infinite norm".

$Eq^n.(4)$ now simplifies to

$$\int |C_a|^2 da = 1 \quad \text{———} \quad (5)$$

In general, if the spectrum of A has both discrete and continuous parts, we have

$$\sum |C_a|^2 + \int |C_a|^2 da = 1 \quad \text{———} \quad (6)$$

Hence, we will write out all delta functions, sums over eigenvalues if the spectrum were discrete.

Hence, $$\psi = \sum_a C_a \phi_a \quad \text{———} \quad (7)$$

and, $$\int \phi_a^* \phi_{a'} d\tau = \delta_{aa'} \quad \text{———} \quad (8).$$

Whenever the spectrum has a continuous part, the summation signs are to be understood as including integrations over the continuous part.

* Closure :-

Any set of functions $\{\phi_a\}$ which is orthonormal and complete has the important property of clouser

$$\sum_a \phi_a(\vec{x})\, \phi_a^*(\vec{x}') = \delta(\vec{x} - \vec{x}') \quad \text{———} \quad (9)$$

This can be prove as follows :

let $$\psi = \sum_m C_m \phi_m \quad \text{———} \quad (10)$$

Multiplying on both the sides by ϕ_n^* and integrating we get

$$\int \phi_n^* \psi \, d\tau = \sum_m C_m \int \phi_n^* \phi_m \, d\tau \quad \text{———} \quad (11)$$

But $\{\phi_n\}$ are orthonormal to each other

Hence, $\phi_n^* \phi_m d\tau = \delta_{m,n}$

$$\therefore \int \phi_n^* \psi \, d\tau = \sum_m C_m \delta_{m,n}$$
$$= C_n$$
$$\therefore C_n = \int \phi_n^* \psi \, d\tau \qquad ------ (12)$$

substituting eqn (12) in (10) we get

$$\psi = \sum_m \left[\int \phi_m^* \psi \, d\tau \right] \phi_m$$
$$= \sum_m \int \left[\phi_m^* (\vec{r}') \psi (\vec{r}') d\tau' \right] \phi_m (\vec{r})$$
$$\therefore \psi (\vec{r}) = \sum_m \left[\int \phi_m^* (\vec{r}') \phi_m (\vec{r}) \right] \psi (\vec{r}') d\tau' \qquad ---- (13)$$

In this eqn $\sum_m \phi_m^* (\vec{r}') \phi_m (\vec{r})$ must be $\delta (\vec{r} - \vec{r}')$ then we must get

$$\psi (\vec{r}) = \int \delta (\vec{r} - \vec{r}') \psi (\vec{r}') d\tau' \qquad --- (14)$$

Here, $\sum_m \phi_m^* (\vec{r}) \phi_m (\vec{r}') = \delta (\vec{r} - \vec{r}')$ is the clouser of $\{\phi_m\}$

Hence in general, the ~~clous~~ closure property of the set of function $\{\phi_a\}$ can be written as

$$\boxed{\sum_a \phi_a (\vec{x}) \phi_a^* (\vec{x}') = \delta (\vec{x} - \vec{x}')} \qquad 15$$

* **Physical Interpretation of eigenvalues, eigenfunctions and expansion coefficients :-**

Suppose A is the dynamical operator of any ~~funct~~ system, In which we are taking A observations. Let ψ be the state of the system. The set of eigen function of operator A be $\{\phi_a\}$.

Then, $$\psi = \sum_a C_a \phi_a \quad \text{—— (1)}$$

where Ca is the coefficients.

$$C_a = \int \phi_a^* \psi \, d\tau \quad \text{—— (2)}$$

For normalization of ψ

$$\sum_a |C_a|^2 = 1 \quad \text{—— (3)}$$

Here we consider ψ is normalized

If ψ is normalized then state of the system be ψ. We get different eigenvalues corresponding to an operator A. Our observation may be any one of them. The proper eigenvalues can be find by taking the ~~average~~ average of eigen values, of the state ψ.

The expectation values of dynamical operator A is given by

$$\langle A \rangle = \int \psi^* A \psi \, d\tau$$

$$= \int \left(\sum_{a'} C_{a'}^* \phi_{a'}^* \right) A \left(\sum_a C_a \phi_a \right) d\tau$$

$$= \sum_a \sum_{a'} C_a C_{a'}^* \int \phi_{a'}^* A \phi_a \, d\tau$$

But $A \phi_a = a \phi_a$ $\therefore$ $\langle A \rangle = \sum_a \sum_{a'} C_a C_{a'}^* a \int \phi_{a'}^* \phi_a \, d\tau$

$$\therefore \langle A \rangle = \sum_a \sum_{a'} C_{a'}^* C_a \, a \, \delta_{aa'}$$

$$= \sum_a |C_a|^2 a \qquad \text{—— (4)}$$

The function ϕ_a are orthonormal. Hence $\delta_{aa'} = 1$ for $a = a'$.

Eq^n (4) states that $\langle A \rangle$ is the weighted average of the eigenvalues a of A. The weight factors are the positive quantities $|C_a|^2$ whose sum is unity.

The physical meaning of these observation is the following:

The result of any measurement A is one of its eigenvalues. The probability that a particular value 'a' comes out as the answer, when the system is in the state ψ is given by $|C_a|^2$. When repeated measurements of A are made on systems in the state ψ the number of times the answer a is obtained is expected to be proportional to $|C_a|^2$. The physical significance of the eigenvalues of any observable is that they are the possible results of measurements of the observable.

The significance of the eigenfunctions can also be seen. Suppose ψ is itself be chosen to be one of the eigenfunctions of A say $\phi_{a'}$. In these case

$$C_a = \int \phi_{a'}^* \phi_a \, d\tau = \delta_{aa'}$$

Thus, $C_a = 1$ for $a = a'$, and zero for all other a.

Hence, the probability $|C_a|^2$ for getting the answer a on measuring A is unity for $a = a'$.

Thus, the eigenfunctions $\phi_{a'}$ of A represents 'a' state in which the observable A has a definite value a'. Expressed differently, the uncertainty in the value of A is zero if the system is in one of the eigenvalues of A.

The interpretation of C_a ~~as a~~ is the probability amplitude and $|C_a|^2$ is a probability density. Hence if we know the coefficients C_a we ~~get~~ can obtain the information about the function ψ. Therefore, considering C_a as a function of a, it is called 'A - space wave function' just as $\psi(\vec{x})$ is called the ~~sp~~ 'coordinate space' or 'configuration space wave function'. We say that C_a and $\psi(\vec{x})$ are different representation of the state. C_a is represented by column matrix as

$$\begin{bmatrix} C_1 \\ C_2 \\ \vdots \\ C_n \end{bmatrix}$$

This matrix is called 'A - representation of the state ψ.

* Momentum Eigenfunctions ; Wave functions in Momentum space :-

⇒ Eigenvalue equation :

The one - dimensional momentum operator is $-i\hbar \frac{d}{dx}$. The eigen value equation is

$$-i\hbar \frac{d\phi_p}{dx} = p\phi_p \quad \text{--- (1)}$$

where p is eigenvalue and ϕ_p is corresponding eigenfunction.

Now in quantum mechanics $p = \hbar k$ — (2)

The eigen function corresponding to k is ϕ_k

Hence, eqn (1) becomes

$$\frac{d\phi_k}{dx} = -\frac{p}{i\hbar}\phi_k = -\frac{\hbar k}{i\hbar}\phi_k$$

$$\therefore \frac{d\phi_k}{dx} = ik\phi_k \qquad (\because i^2 = -1)$$

$$\therefore \frac{d\phi_k}{\phi_k} = ik\,dx$$

Integrating this relation, we get

$$\ln\phi_k = ikx + C_1$$

$$\therefore \phi_k = e^{ikx}\cdot e^{C_1} = Ce^{ikx}$$

$$\therefore \boxed{\phi_k = Ce^{ikx}} \quad ----- (3)$$

where C is constant of integration. This constant can be determined by normalization.

⇒ Normalization of momentum eigen functions:-

From eqn (3) it is clear that momentum eigen function is non-normalizable. Then we have to use box normalization or δ-function normalization.

(a) Box normalization:

Let us consider particle is confined within a box of length L. Taking one end of the box as a origin.

$$\therefore \int_0^L \phi_k^*(x)\,\phi_k(x)\,dx = C^2\int_0^L e^{-ikx}e^{ikx}dx$$

$$= C^2\int_0^L dx$$

$$= C^2 L$$

For normalization it should be 1

$$\therefore C^2 = 1/L \quad \therefore C = 1/\sqrt{L}$$

Hence eq^n (3) becomes

$$\boxed{\phi_k = \frac{1}{\sqrt{L}} e^{ikx}} \quad \text{-----} (4)$$

This is a box normalized momentum eigen functions.

For three-dimensional

$$\phi_{\vec{k}} = \frac{1}{L^{3/2}} e^{i\vec{k}\cdot\vec{r}} \quad \text{---} (5)$$

(b) δ - function normalization:

For box-normalization following condition must be satisfied.

$$\phi_k(x=0) = \phi_k(x=L)$$

$$\therefore \frac{1}{\sqrt{L}} e^0 = \frac{1}{\sqrt{L}} e^{ikL}$$

$$\therefore e^{ikL} = 1$$

Hence $$\boxed{k = \frac{2\pi}{L} n} \quad \text{-----} (6)$$

where $n = 0, \pm 1, \pm 2 \ldots$

Eq^n (6) represent that the momentum of the particle is descreate. It is not true. In actual practice, the momentum must be continuous. ~~Hence~~ If the eigen values are continum then we take δ - function normalization. Hence, we must find a normalization factor in such that

$$\int_{-\infty}^{\infty} \phi_{k'}^* \phi_{k'} \, dx = \delta(k-k') \quad \text{———} (7)$$

But $\phi_k = C e^{ikx}$

$\phi_{k'} = C e^{ik'x}$

$$\therefore \int_{-\infty}^{\infty} \phi_{k'}^{*} \phi_{k} \, dx = C^2 \int_{-\infty}^{\infty} e^{-ik'x} e^{ikx} dx$$

$$= C^2 \int_{-\infty}^{\infty} e^{i(k-k')x} dx$$

$$= \lim_{g \to \infty} C^2 \int_{-g}^{+g} e^{i(k-k')x} dx$$

$$= \lim_{g \to \infty} C^2 \left[\frac{e^{i(k-k')x}}{i(k-k')} \right]_{-g}^{g}$$

$$= \lim_{g \to \infty} C^2 \left[\frac{e^{i(k-k')g} - e^{-i(k-k')g}}{i(k-k')} \right]$$

$$= \lim_{g \to \infty} \frac{2C^2}{k-k'} \left[\frac{e^{i(k-k')g} - e^{-i(k-k')g}}{2i} \right]$$

$$= \lim_{g \to \infty} 2C^2 \left[\frac{\sin(k-k')g}{(k-k')} \right]$$

For δ- function normalization this must be $\delta(k-k')$

$$\therefore \lim_{g \to \infty} 2C^2 \left[\frac{\sin(k-k')g}{k-k'} \right] = \delta(k-k') \quad \text{—— (8)}$$

But $\delta(x) = \lim_{g \to \infty} \frac{\sin gx}{\pi x}$ - - - - (9)

In this case, $\delta(k-k') = \lim_{g \to \infty} \frac{\sin g(k-k')}{\pi(k-k')}$ - - - - (10)

~~Now~~ $\therefore$ Eqn (8) can be written as

$$\lim_{g \to \infty} 2C^2 \pi \left[\frac{\sin(k-k')g}{\pi(k-k')} \right] = \delta(k-k')$$

$$\therefore 2\pi C^2 \delta(k-k') = \delta(k-k')$$

$$\therefore C = \frac{1}{(2\pi)^{1/2}} \quad \text{- - - - - (11)}$$

Hence, in δ- function normalization, the normalization constant is $\frac{1}{(2\pi)^{1/2}}$.

Hence, by the δ-function, normalized momentum eigen function is given by

$$\phi_k = \frac{1}{(2\pi)^{1/2}} e^{ikx} \quad \text{——— (12)}$$

In three-dimensions

$$\phi_{\vec{k}} = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{x}} \quad \text{.... (13)}$$

* Closure property of momentum eigen functions:

(a) Box normalised eigen functions:

The ~~clouse~~ closure ~~pea~~ property is

$$\sum_{n=-\infty}^{\infty} \phi_k^*(x)\,\phi_k(x') = \delta(x-x') \quad \text{——— (14)}$$

But $k = \frac{2\pi}{L}n$ $\qquad \phi_k = \frac{1}{\sqrt{L}} e^{ikx}$

$$\therefore \sum_{n=-\infty}^{\infty} \frac{1}{L} e^{-i\frac{2\pi}{L}nx} \cdot e^{i\frac{2\pi}{L}nx'}$$

$$= \sum_{n=-\infty}^{\infty} \frac{1}{L} e^{-i\frac{2\pi}{L}n(x-x')} \quad \text{——— (15)}$$

$$= \lim_{N\to\infty} \frac{1}{L} \sum_{n=-N}^{N} e^{-i\frac{2\pi}{L}n(x-x')}$$

This is a physical series. Its first component is

$$a = e^{i\frac{2\pi}{L}N(x-x')}$$

and the ratio of two remaining terms is

$$p = \frac{e^{+i\frac{2\pi}{L}(+N+1)(x-x')}}{e^{+i\frac{2\pi}{L}(+N+2)(x-x')}} = e^{-i\frac{2\pi}{L}(x-x')}$$

Now, the sol^n of series $S = a + ap + ap^2 + \dots + ap^{n-1} = a\frac{1-p^n}{1-p}$

$$\therefore \lim_{N\to\infty} \frac{1}{L}\sum_{n=-N}^{n=+N} e^{-i\frac{2\pi}{L}n(x-x')} = \lim_{N\to\infty} \frac{1}{L} e^{i\frac{2\pi}{L}N(x-x')} \frac{\left[1-e^{-i\frac{2\pi}{L}(2N+1)(x-x')}\right]}{\left[1-e^{-i\frac{2\pi}{L}(x-x')}\right]}$$

$$= \lim_{N\to\infty} \frac{1}{L} e^{i\frac{2\pi}{L}N(x-x')} \cdot e^{-i\frac{\pi}{L}(2N+1)(x-x')} \frac{\left[e^{i\frac{\pi}{L}(2N+1)(x-x')} - e^{-i\frac{\pi}{L}(2N+1)(x-x')}\right]}{e^{-i\frac{\pi}{L}(x-x')}\left[e^{i\frac{\pi}{L}(x-x')} - e^{-i\frac{\pi}{L}(x-x')}\right]}$$

$$= \lim_{N\to\infty} \frac{1}{L}\left[e^{i\frac{\pi}{L}(2N+1)(x-x')} \cdot e^{-i\frac{\pi}{L}(2N+1)(x-x')}\right] \left[\frac{\sin\frac{\pi}{L}(2N+1)(x-x')}{\left[\sin\frac{\pi}{L}(x-x')\right]}\right]$$

$$= \lim_{N\to\infty} \frac{1}{L} \frac{\left[\sin(2N+1)(x-x')\pi/L\right]}{\left[\sin(x-x')\pi/L\right]}$$

$$= \frac{\pi}{L}\cdot\delta\left(\frac{\pi}{L}(x-x')\right) = \frac{\pi}{L}\cdot\frac{L}{\pi}\,\delta(x-x')$$

$$= \delta(x-x')$$

$$\therefore \sum_{n=-\infty}^{\infty} \phi_k^*(x)\phi_k(x') = \delta(x-x') \quad \text{——— (16)}$$

(b) <u>δ- function normalized eigen functions:-</u>

We know that

$$\phi_k = \frac{1}{(2\pi)^{1/2}} e^{ikx} \quad \text{——— (17)}$$

$$\therefore \sum_k \phi_k(x)\phi_k^*(x') = \sum_k \frac{1}{2\pi} e^{ik(x-x')}$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik(x-x')}dk \quad (\because k \text{ is continuum})$$

$$= \frac{1}{2\pi}\, 2\pi\, \delta(x-x')$$

$$\therefore \sum_k \phi_k(x)\phi_k^*(x') = \delta(x-x') \quad \text{——— (18)}$$

because $\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}\, dk$.

In three dimensions

$$\sum_{\vec{k}} \phi_{\vec{k}}(\vec{r})\, \phi^*_{\vec{k}}(\vec{r}\,') = \delta(\vec{r} - \vec{r}\,') \quad \text{—— (19)}$$

Now, momentum eigen functions are orthogonal to each other and its norm is unity. Hence we get a complete set of the function $\{\phi_k(\vec{r})\}$.

$$\therefore \quad \psi(\vec{r}) = \sum_{\vec{k}} C(\vec{k})\, \phi_{\vec{k}}(\vec{r}) \quad \text{—— (20)}$$

Now, multiplying on both the sides by $\phi^*_{\vec{k}'}(\vec{r})$ and Integrating we get

$$\int \phi^*_{\vec{k}'}(\vec{r})\, \psi(\vec{r})\, d^3r = \sum_{\vec{k}} C(\vec{k}) \int \phi^*_{\vec{k}'} \phi_k\, d^3r$$

$$= \sum_{\vec{k}} C(\vec{k})\, \delta(\vec{k} - \vec{k}')$$

$$= \int C(\vec{k})\, \delta(\vec{k} - \vec{k}')\, d^3k$$

$$(\because k = k')$$

$$= C(\vec{k}')$$

$$\therefore \quad C(\vec{k}) = \int \phi^*_{\vec{k}}(\vec{r})\, \psi(\vec{r})\, d^3r \quad \text{—— (21)}$$

Now, $\phi^*_{\vec{k}}(\vec{r}) = \frac{1}{(2\pi)^{3/2}}\, e^{-i\vec{k}\cdot\vec{r}}$

$$\therefore \quad C(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \int \psi(\vec{r})\, e^{-i\vec{k}\cdot\vec{r}}\, d^3r \quad \text{—— (22)}$$

For continuous distribution eqn (20) can be written as

$$\psi(\vec{r}) = \int C(\vec{k})\, \phi_{\vec{k}}(\vec{r})\, d^3k \quad \text{—— (24)}$$

where $\phi_{\vec{k}} = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}}$

$$\therefore \psi(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \int C(\vec{k})\, e^{i\vec{k}\cdot\vec{r}}\, d^3r \quad \text{—— (25)}$$

Eq^n (22) and (24) are Fourier transform to each other.

If we $\vec{p} = \hbar\vec{k}$ by $\vec{k}$ then we get

$$\psi(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}} \int C(\vec{p})\, e^{i\vec{p}\cdot\vec{r}/\hbar}\, d^3p \quad \text{—— (26)}$$

and,
$$C(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int \psi(\vec{r})\, e^{-i(\vec{p}\cdot\vec{r})/\hbar}\, d^3r \quad \text{—— (27)}$$

Eq^n (26) shows that if $\psi(r)$ represent the state of the system of observable momentum p then probability to get the momentum p is $|C(\vec{p})|^2$. It is given by eq^n (27). $\psi(\vec{r})$ is the Fourier transform of $C(\vec{k})$.

The expectation value of any function on momentum is

$$\langle f(\vec{p})\rangle = \int |C(\vec{p})|^2 f(\vec{p})\, d^3p \quad \text{—— (28)}$$

$C(\vec{p})$ may be called the momentum space wave function. It gives probability amplitude and $|C(\vec{p})|^2$ the probability density. $C(\vec{p})$ contains the same information as the configuration space wave function $\psi(\vec{r})$. In momentum space, the dynamical variables would be represented by operator which act on $C(\vec{p})$. The position and momentum are represented by

$$\boxed{\vec{X}_{op} = i\hbar\nabla_{\vec{p}}}, \quad \text{—— (29)}$$

and,
$$\boxed{\vec{P}_{op} = \vec{p}} \quad \text{—— (30)}$$

where $\nabla_{\vec{p}} = \left(\frac{\partial}{\partial p_x}, \frac{\partial}{\partial p_y}, \frac{\partial}{\partial p_z}\right)$.

* Eigen value equation of position operator in momentum space:

The eigenvalue eq^n of position operator in momentum space is given by

$$\vec{r}_{op}\, C(\vec{p}) = \vec{r}\, C(\vec{p}) \quad \text{---- (31)}$$

$$\therefore i\hbar\vec{\nabla}_{\vec{p}}\, C(\vec{p}) = \vec{r}\, C(\vec{p}) \quad \text{—— (32)}$$

but $C(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int \psi(\vec{r})\, e^{-i(\vec{p}\cdot\vec{r})/\hbar}\, d^3r$ —— (33)

$$\therefore\ i\hbar \nabla_{\vec{p}} \left[\frac{1}{(2\pi\hbar)^{3/2}} \int \psi(\vec{r})\, e^{-i(\vec{p}\cdot\vec{r})/\hbar}\, d^3r \right]$$

$$= (i\hbar)\, \frac{-ir}{\hbar} \left[\frac{1}{(2\pi\hbar)^{3/2}} \int \psi(\vec{r})\, e^{-i(\vec{p}\cdot\vec{r})/\hbar}\, d^3r \right]$$

$$= \vec{r}\, C(\vec{p})$$

$$\therefore \boxed{i\hbar \nabla_{\vec{p}} C(\vec{p}) = \vec{r}\, C(\vec{p})} \quad \text{—— (34)}$$

Ex: Suppose particle is represented by the wave function $\psi(x) = (\sqrt{\pi})^{-1/2} e^{-x^2/2}$. then find the probability of wave vector k.

$-\frac{1}{2}(x^2 + 2ikx + i^2k^2) - \frac{k^2}{2}$

$-\frac{x^2}{2} - \frac{2ikx}{2} + \frac{k^2}{2} - \frac{k^2}{2}$

Sol^n: $C(k) = \frac{1}{(2\pi)^{1/2}} \int \psi(x)\, e^{-ikx}\, dx$

$$= \frac{1}{(2\pi)^{1/2}} (\sqrt{\pi})^{-1/2} \int_{-\infty}^{\infty} e^{-x^2/2}\, e^{-ikx}\, dx$$

$$= \frac{1}{(2\pi)^{1/2}} \frac{1}{(\pi)^{1/4}} \int_{-\infty}^{\infty} e^{-\frac{1}{2}(x+ik)^2} \cdot e^{-k^2/2}\, dx$$

$$= \frac{1}{(2\pi)^{1/2}} \frac{1}{(\pi)^{1/4}}\, e^{-k^2/2} \int_{-\infty}^{\infty} e^{-\frac{1}{2}(x+ik)^2}\, dx$$

$$= \frac{e^{-k^2/2}\ \sqrt{2\pi}}{(2\pi)^{1/2} (\pi)^{1/4}}$$

$e^{-\frac{k^2}{2}}\, e^{-k^2/2}$

$e^{-2k^2/2}$

$$= \frac{e^{-k^2/2}}{(\sqrt{\pi})^{1/2}}$$

$$C(k) = \frac{1}{(\sqrt{\pi})^{1/2}} e^{-k^2/2}$$

$$\boxed{|C(k)|^2 = \frac{1}{\sqrt{\pi}} e^{-k^2}}$$

This is the probability of wave vector $\vec{k}$.

* ## The Uncertainty Principle :

The uncertainty in the value of quantum mechanical observables also defined in the same way of uncertainty principle. If A is an observable and $\langle A \rangle$ ~~is~~ its expectation or mean value in the state ψ then deviation is $A - \langle A \rangle$. and is the self adjoint operator. The square of this deviation gives the uncertainty of A, it is denoted by ΔA.

$$\therefore (\Delta A)^2 = \langle (A - \langle A \rangle)^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2 \quad —— (1)$$

Similarly for other variable B we can write

$$(\Delta B)^2 = \langle (B - \langle B \rangle)^2 \rangle \quad ------ (2).$$

Here ΔA and ΔB are not operator., but $A - \langle A \rangle$ is the square root of mean square operator. Now this operator is represented by deviation operator D_a and D_b.

$$\therefore D_a = A - \langle A \rangle \quad ------ (3)$$

$$D_b = B - \langle B \rangle \quad ------ (4)$$

Now ~~u~~sing the positivity property of operators

$$\langle (D_a - i\lambda D_b)(D_a + i\lambda D_b) \rangle \geqslant 0 \quad --- (5)$$

λ is a real parameter.

Let we expand the product as

$$\langle D_a^2 + i\lambda D_a D_b - i\lambda D_b D_a + \lambda^2 D_b^2 \rangle$$

Now taking the diffⁿ w.r.t λ and equating to zero we get

$$\langle 0 + i D_a D_b - i D_b D_a + 2\lambda D_b^2 \rangle = 0$$

$$\therefore \langle i[D_a, D_b] \rangle + 2\lambda \langle D_b^2 \rangle = 0$$

$$\therefore \lambda = \frac{\langle -i[D_a, D_b] \rangle}{2\langle D_b^2 \rangle} \quad ---- (6)$$

Substituting this value of λ in eqn (5) we get

$$\left\langle D_a^2 + i\frac{\langle -i[D_a, D_b]\rangle}{2\langle D_b^2\rangle} D_a D_b - i\frac{\langle -i[D_a, D_b]\rangle}{2\langle D_b^2\rangle} D_b D_a + \frac{\langle -i[D_a,D_b]\rangle^2}{4\langle D_b^2\rangle^2} D_b^2\right\rangle \geq 0$$

$$\left\langle D_a^2 + \frac{\langle [D_a, \cancel{D_b}]\rangle}{2\langle \cancel{D_b^2}\rangle} D_a D_b - \frac{\langle [D_a, \cancel{D_b}]\rangle}{2\langle \cancel{D_b^2}\rangle} D_b D_a + \frac{\langle [D_a, D_b]\rangle^2}{4\langle D_b^2\rangle}\right\rangle \geq 0$$

$$\therefore \langle D_a^2\rangle + \frac{\langle [D_a, D_b]\rangle \langle [D_a, D_b]\rangle}{\langle 4 D_b^2\rangle} \geq 0$$

$$\therefore 4\langle D_a^2\rangle\langle D_b^2\rangle + \langle [D_a, D_b]\rangle^2 \geq 0 \qquad \text{------ (7)}$$

From eqn (3), we have

$$D_a^2 = A^2 - 2A\langle A\rangle + \langle A\rangle^2$$

$$\therefore \langle D_a^2\rangle = \langle A^2\rangle - 2\langle A\rangle\langle A\rangle + \langle A\rangle^2$$

$$= \langle A^2\rangle - 2\langle A\rangle^2 + \langle A\rangle^2$$

$$= \langle A^2\rangle - \langle A\rangle^2 \qquad \text{------ (8)}$$

||ly,

$$\langle D_b^2\rangle = \langle B^2\rangle - \langle B\rangle^2 \qquad \text{---- (9)}$$

Now, $[D_a, D_b] = [A - \langle A\rangle, B - \langle B\rangle]$

$$= [A, B] - [\langle A\rangle, B] - [A, \langle B\rangle] + [\langle A\rangle, \langle B\rangle]$$

$$= [A, B] \qquad \text{------- (10)}$$

other terms vanishes by the property of commutators.

Now, using eqn. (8), (9), (10) in (7), we get

$$4[\langle A^2\rangle - \langle A\rangle^2][\langle B^2\rangle - \langle B\rangle^2] + \langle [A, B]\rangle^2 \geq 0$$

Using eqn. (1) & (2) we can write

$$4(\Delta A)^2(\Delta B)^2 + \langle [A, B]\rangle^2 \geq 0$$

$$\therefore 4(\Delta A)^2(\Delta B)^2 \geq -\langle [A, B]\rangle^2$$

$$\therefore (\Delta A)^2(\Delta B)^2 \geq -\frac{1}{4}\langle [A, B]\rangle^2 \qquad \text{---- (11)}$$

$$\therefore (\Delta A)(\Delta B) \geq -\frac{1}{2}\langle [A, B]\rangle \qquad \text{------ (12)}$$

This is the product of uncertainty in A and B and is ~~of~~ of the order of commutator $[A,B]$ Eqn. (12) gives the general statement of the uncertainty principle for any pair of observables A, B.

If A, B are a canonically conjugate pair of operators, it is characterized by

$$[A,B] = i\hbar \quad \text{——— (13)}$$

then,
$$(\Delta A)(\Delta B) \geq \frac{1}{2}\hbar \quad \text{- - — (14)}$$

Here, sign is not important.

Now, $[x, p_x] = i\hbar$

$$\therefore \left.\begin{aligned} (\Delta x)(\Delta p_x) &= \frac{\hbar}{2} \\ (\Delta y)(\Delta p_y) &= \frac{\hbar}{2} \\ (\Delta z)(\Delta p_z) &= \frac{\hbar}{2} \end{aligned}\right\} \quad \text{—— (15)}$$

Ex: Prove that the same state of all the component of $\vec{L}$ is impossible.

Now, we have $[L_x, L_y] = i\hbar L_z$ ---- (16)

Now, consider a function ϕ which satisfies both the eigen equation of L_x and L_y.

$$\therefore \quad L_x\phi = m_x\phi \quad \text{—— (17)}$$

$$\text{and,} \quad L_y\phi = m_y\phi \quad \text{—— (18)}$$

Now, multiplying eqn (17) by L_y and (18) by L_x and subtracting we get,

$$L_yL_x\phi = L_y m_x\phi$$
$$L_xL_y\phi = L_x m_y\phi$$

$$(L_yL_x - L_xL_y)\phi = m_xL_y\phi - m_yL_x\phi$$

$$\therefore (L_xL_y - L_yL_x)\phi = m_yL_x\phi - m_xL_y\phi$$
$$= m_ym_x\phi - m_xm_y\phi = 0$$

$$\therefore [L_x, L_y]\phi = 0 \qquad \text{—— (19)}$$

Now, comparing this eqn (19) with (16) we get

$$[L_x, L_y]\phi = i\hbar L_z\phi = 0$$

$$\therefore L_z\phi = 0 \qquad \text{—— (20)}$$

Similarly if we repeat the calculation for L_x and L_y, we must have

$$L_x\phi = 0$$

$$\text{and } L_y\phi = 0$$

Hence, if any two components of angular momentum have same eigen state and applying this eigen state on third component, then results will be zero. Thus, the eigen state of all the three components of angular momentum will not be same.

* States with minimum value for uncertainty product :-

We have obtain the uncertainty principle $(\Delta x)(\Delta p) \geq \frac{1}{2}\hbar$ using the positive property

$$\langle (D_a - i\lambda D_b)(D_a + i\lambda D_b) \rangle \geq 0 \qquad \text{—— (1)}$$

If the L.H.S of this eqn becomes zero then the product of uncertainty will be zero. For this we must have the state function $\psi(x)$ such that

$$(D_a + i\lambda D_b)\psi = 0 \qquad \text{—— (2)}$$

If $A = x$, $B = -i\hbar \frac{d}{dx}$ —— (3)

then,

$$D_a = x - \langle x \rangle \qquad \text{—— (4)}$$

$$D_b = p_x - \langle p_x \rangle \qquad \text{—— (5)}$$

$$\langle D_b^2 \rangle = \langle p_x^2 \rangle - \langle p_x \rangle^2 \qquad \text{—— (6)}$$

$$(\Delta p_x)^2 = \langle p_x^2 \rangle - \langle p_x \rangle^2 \qquad \text{—— (7)}$$

We also know that, $\lambda = \dfrac{-i\langle[x, p_x]\rangle}{2(\Delta p_x)^2}$ —— (8)

Here, $[D_a, D_b] = [A, B] = [x, p_x]$

$$\therefore \lambda = \frac{(-i)(i\hbar)}{2(\Delta p_x)^2} \quad \text{—— (9)}$$

Substituting eqns. (4), (5) & (9) in eqn (2) we get

$$\left[x - \langle x\rangle + \frac{(i)(-i)(i\hbar)}{2(\Delta p_x)^2}(p_x - \langle p_x\rangle)\right]\psi = 0$$

Substituting $p_x = -i\hbar\frac{d}{dx}$ and arranging the terms we get

$$\left[x - \langle x\rangle + \frac{i\hbar}{2(\Delta p_x)^2}\left(-i\hbar\frac{d}{dx} - \langle p_x\rangle\right)\right]\psi = 0$$

$$\left[x - \langle x\rangle + \frac{\hbar^2}{2(\Delta p_x)^2}\frac{d}{dx} - \frac{i\hbar}{2(\Delta p_x)^2}\langle p_x\rangle\right]\psi = 0$$

$$\left[\frac{\hbar^2}{2(\Delta p_x)^2}\frac{d}{dx} + x - \langle x\rangle - \frac{i\hbar}{2(\Delta p_x)^2}\langle p_x\rangle\right]\psi = 0$$

$$\therefore \frac{d\psi}{dx} + \left\{\frac{2(\Delta p_x)^2}{\hbar^2}(x - \langle x\rangle) - \frac{i\langle p_x\rangle}{\hbar}\right\}\psi = 0 \quad \text{—— (10)}$$

$$\therefore \frac{d\psi}{dx} = -\left\{\frac{2(\Delta p_x)^2}{\hbar^2}(x - \langle x\rangle) - \frac{i\langle p_x\rangle}{\hbar}\right\}\psi$$

$$\therefore \frac{d\psi}{\psi} = -\left\{\frac{2(\Delta p_x)^2}{\hbar^2}(x - \langle x\rangle) - \frac{i\langle p_x\rangle}{\hbar}\right\}dx$$

Integrating on both the sides we get

$$\ln\psi = -\left\{\frac{2(\Delta p_x)^2}{\hbar^2}\left(\frac{x^2}{2} - \langle x\rangle x\right) - \frac{i\langle p_x\rangle}{\hbar}x\right\}$$

$$= -\left\{\frac{(\Delta p_x)^2}{\hbar^2}(x^2 - 2x\langle x\rangle) - \frac{i\langle p_x\rangle}{\hbar}x\right\}$$

$$= -\left\{\frac{(\Delta p_x)^2}{\hbar^2}(x - \langle x\rangle)^2 - \frac{(\Delta p_x)^2}{\hbar^2}\langle x\rangle^2 - \frac{i\langle p_x\rangle}{\hbar}x\right\}$$

$$\therefore \psi = N \exp\left\{ -\frac{(\Delta p_x)^2}{\hbar^2}(x - \langle x \rangle)^2 - \frac{i\langle p_x \rangle}{\hbar} x \right\} \qquad \text{--- (11)}$$

Here the ~~constant~~ factor $\frac{(\Delta p_x)^2}{\hbar^2}$ is contain in constant N.

The wave function is normalised

i.e $\int |\psi|^2 dx = 1$ if N is chosen as

$$N = \left[\frac{2(\Delta p_x)^2}{\pi \hbar^2} \right]^{1/4} \qquad \text{--- (12)}$$

$$\therefore |\psi|^2 = \left(\frac{2(\Delta p_x)^2}{\pi \hbar^2} \right)^{1/2} \exp\left[-\frac{2(\Delta p_x)^2}{\hbar^2} (x - \langle x \rangle)^2 \right] \qquad \text{--- (13)}$$

Eq^n (11) gives the normalized wave function for which $(\Delta x)(\Delta p_x)$ has the minimum value $\hbar/2$. Note that ψ has the form of a Gaussian function 'modulated' by the oscillatory factor $\exp\left[\frac{i\langle p_x \rangle}{\hbar} x \right]$.

For minimum uncertainty

$$(\Delta x)(\Delta p_x) = \hbar/2$$

$$\therefore \Delta p_x = \frac{\hbar}{2(\Delta x)} \qquad \text{--- (14)}$$

Substituting this value of Δp_x in eq^n (13) we get

$$|\psi|^2 = \left(\frac{2\hbar^2}{4(\Delta x)^2 \pi \hbar^2} \right)^{1/2} \exp\left[-\frac{2\hbar^2}{4(\Delta x)^2 \hbar^2} (x - \langle x \rangle)^2 \right]$$

$$\therefore |\psi|^2 = \left[2\pi (\Delta x)^2 \right]^{-1/2} \exp\left[-\frac{(x - \langle x \rangle)^2}{2(\Delta x)^2} \right] \qquad \text{--- (15)}$$

Since $|\psi|^2$ is negligibly small outside a region having dimensions of the order $\Delta x = (\hbar / 2\Delta p_x)$, the wave function (11) is said to describe a minimum uncertainty wave packet.

* Commuting Observables; Removal of Degeneracy :-

Consider an eigen value eqn

$$A\phi_a = a\phi_a \quad \text{--- (1)}$$

Let us consider ~~an~~ another operator B which commute with A. Now operate B on both the sides we have

$$BA\phi_a = aB\phi_a \quad \text{--- (2)}$$

But $BA = AB$

$$\therefore A(B\phi_a) = a(B\phi_a) \quad \text{--- (3)}$$

Thus not only ϕ_a, but $B\phi_a$ also is an eigenstate of A belonging to the same eigenvalue a. If 'a' happens to be a non-degenerate eigenvalue, there is only one eigenfunction belonging to it and hence $B\phi_a$ must be a constant multiple of ϕ_a, say

$$B\phi_a = b\phi_a \quad \text{--- (4)}$$

This means that ϕ_a is also an eigenfunction of B, belonging to eigenvalues b. Thus any eigenfunction belonging to a non-degenerate eigenvalue of ~~either of~~ a pair of commuting operator A, B is necessarily an eigenfunction of the other operator.

It is possible to choose a basic set of r eigenfunction in such a way that each of them is an eigenfunction of B. In this manner one can obtain a completeset of simultaneous eigenfunctions ϕ_{ab} for any pair of commuting observable A, B. If the r independent eigenfunctions belonging to a given degenerate eigenvalue 'a' are characterized by r distinct value of b, then we say that the degeneracy of a is completely removed.

If it is not removed then we have to introduce another observables C.

$\phi_{abc\ldots}$ and $\phi_{a'b'c'\ldots}$ are identical if and only if $a=a'$, $b=b'$, $c=c'$, ... It is obvious that if each $\phi_{abc\ldots}$ is ~~indu~~ individually normalized, the set of all such simultaneous eigenfunctions forms an orthonormal set

$$\int \phi^*_{abc\ldots}\, \phi_{a'b'c'\ldots}\, d\tau = \delta_{aa'}, \delta_{bb'}, \delta_{cc'}, \ldots \qquad (5).$$

* **Evolution of system with time; Constants of the motion :-**

The time dependent ~~Stat~~ Schrodinger equation is

$$i\hbar \frac{\partial \psi}{\partial t}(\vec{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) + V(\vec{r})\psi(\vec{r},t) \qquad (1)$$

Here, $-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}) = H_{op}$

$$\therefore \quad i\hbar\frac{\partial\psi}{\partial t} = H_{op}\psi \qquad (2)$$

H_{op} is called Hamiltonian operator. ψ is a function of $\vec{r}$ and t. The solⁿ of eqⁿ (1) is

$$\psi(\vec{r},t) = u(\vec{r})\,\phi(t) \qquad (3)$$

where, $\phi(t) = N e^{-iEt/\hbar}$ — (4)

The expectation value of operator does not depends on time. For example operator A_{op}

$$\langle A \rangle = \int \psi^*(\vec{r},t)\, A_{op}\, \psi(\vec{r},t)\, d\tau$$

$$= \int u^*(\vec{r})\,\phi^*(t)\, A_{op}\, u(\vec{r})\,\phi(t)\, d\tau$$

$$= \int u^*(\vec{r})\, e^{iEt/\hbar}\, A_{op}\, e^{-iEt/\hbar}\, u(\vec{r})\, d\tau$$

Hence if an operator is not depends on time, then

$$\langle A \rangle = \int u^*(\vec{r})\, A_{op}\, u(\vec{r})\, d\tau \qquad (5)$$

* **Postulate – 4 :-** The state ψ varies with time in a manner determined by the Schrodinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = H_{op}\psi \qquad \text{— (1)}$$

where H_{op} is the Hamiltonian operator. The basic dynamical variables $\vec{r}$ and $\vec{p}$ do not change with time.

Consider operator A_{op} which are explicitly time dependent.

$$\frac{d}{dt}\langle A(\vec{r},\vec{p},t)\rangle = \frac{d}{dt}\int \psi^*(\vec{r},t)\, A_{op}\, \psi(\vec{r},t)\, d\tau$$

$$= \int \frac{\partial \psi^*}{\partial t} A(\vec{r},\vec{p},t)\psi\, d\tau + \int \psi^* \frac{\partial A_{op}}{\partial t}\psi\, d\tau + \int \psi^* A_{op}\frac{\partial \psi}{\partial t}\, d\tau \qquad \text{— (2)}$$

But, $$i\hbar \frac{\partial \psi}{\partial t} = H_{op}\psi \qquad \text{— (3)}$$

and, $$-i\hbar \frac{\partial \psi^*}{\partial t} = (H_{op}\psi)^* \qquad \text{— (4)}$$

Using eqn. (3) & (4) in eqn (2) we have

$$\frac{d}{dt}\langle A\rangle = \int -\frac{1}{i\hbar}(H_{op}\psi)^* A_{op}\psi\, d\tau + \int \psi^* \frac{\partial A_{op}}{\partial t}\psi\, d\tau + \int \psi^* A_{op}\left(\frac{1}{i\hbar}H_{op}\psi\right) d\tau$$

But H_{op} is Hermitian

$$\therefore \frac{d}{dt}\langle A\rangle = \int -\frac{1}{i\hbar}\psi^* H_{op} A_{op}\psi\, d\tau + \int \psi^* \frac{\partial A_{op}}{\partial t}\psi\, d\tau + \int \psi^* A_{op}\frac{1}{i\hbar}H_{op}\psi\, d\tau$$

$$\therefore \frac{d}{dt}\langle A\rangle = \int \psi^* \left\{\frac{1}{i\hbar}[A_{op}, H_{op}] + \frac{\partial A_{op}}{\partial t}\right\}\psi\, d\tau \qquad \text{— (5)}$$

Thus, the rate of change of the expectation value of any dynamical variable A may be obtained as the expectation value of $(i\hbar)^{-1}[A, H] + \frac{\partial A}{\partial t}$. This operator may be taken to represent the dynamical variable $\frac{dA}{dt}$.

$$\therefore \left(\frac{dA}{dt}\right)_{op} = \frac{1}{i\hbar}[A_{op}, H_{op}] + \frac{\partial A_{op}}{\partial t} \qquad \text{— (6)}$$

If A is any dynamical variable which is not explicitly time-dependent then $\frac{dA_{op}}{dt} = 0$ and it commutes with H, then $\langle A\rangle$ is independent of time. Such A is said to be a <u>conserved quantity</u> or <u>constant of motion</u>.