B.Sc. (Semester - 6)

Subject: Physics

Course: US06CPHY21

Quantum Mechanics

UNIT – II General Formalism of Wave Mechanics

The Schrödinger Equation and Probability for N-Particle System:

A system of N particles is represented by the position and momentum variables $\vec{X}_1, \vec{X}_2, \dots, \vec{X}_N$ and $\vec{p}_1, \vec{p}_2, \dots, \vec{p}_N$. Its energy is given by

$$E = H(\vec{X}_1, \vec{X}_2, \dots, \vec{X}_N, \vec{p}_1, \vec{p}_2, \dots, \vec{p}_N, t)$$
 ... (2.1)

The operators are

$$E \to i\hbar \frac{\partial}{\partial t}, \quad \vec{p}_i \to -i\hbar \vec{\nabla}_i \qquad ... (2.2)$$

$$(i = 1, 2,N)$$

where,

$$\vec{\nabla}_i = \left(\frac{\partial}{\partial x_i}, \frac{\partial}{\partial y_i}, \frac{\partial}{\partial z_i}\right)$$

These operators have to act on the wave function Ψ . The 3N coordinates of the N particles can be taken as the coordinates of a single point in a 3N- dimensional space. Such a space is called the configuration space.

The wave equation for N-paricle system can be written as

$$i\hbar \frac{\partial \Psi(\vec{X}_{1}, \vec{X}_{2}, \dots, \vec{X}_{N}, t)}{\partial t}$$

$$= H(\vec{X}_{1}, \vec{X}_{2}, \dots, \vec{X}_{N}, -t\hbar \vec{\nabla}_{1}, -t\hbar \vec{\nabla}_{2}, \dots, \dots, -t\hbar \vec{\nabla}_{N}, t)\Psi(\vec{X}_{1}, \vec{X}_{2}, \dots, \vec{X}_{N}, t) \qquad \dots (2.3)$$

This is the general form of the Schrodinger equation.

The Fundamental Postulates of Wave Mechanics:

(a) Representation of states:

Postulate: 1 "The state of a quantum mechanical system is described or represented by a wave function $\Psi(\vec{X},t)$ "

Postulate: 2 The superposition principle:

If Ψ_1 and Ψ_2 are wave functions for any two states of a given system then corresponding to every linear combination $(C_1\Psi_1+C_2\Psi_2)$ of the two functions, there exists a state of the system.

This is a fundamental principal of quantum mechanics to which there is no correspondence in classical mechanics. It is the possibility of superposition which makes interference phenomena possible.

The scalar product of ϕ and Ψ is defined as

$$(\phi, \Psi) = \int \phi^*(\vec{X}) \Psi(\vec{X}) d\tau \qquad \dots (2.4)$$

This follows that,

$$(\phi, \Psi) = (\Psi, \phi)^*$$

$$(\phi, C\Psi) = C(\phi, \Psi), \quad and \quad (C\phi, \Psi) = C^*(\phi, \Psi)$$

The norm of

$$\Psi = (\Psi, \Psi) \ge 0$$

(b) Representation of dynamical variables; Expectation values, Observables: Postulates: 3

Each dynamical variable $A(\vec{X}, \vec{p})$ is represented in quantum mechanics by a linear operator

$$A_{op} = A(\vec{X}_{op}, \vec{p}_{op}) = A(\vec{X}, -i\hbar \vec{\nabla})$$

- \blacktriangleright The operator acts on the wave functions of the system. The effect of an operator A on a wave function Ψ is to convert into another wave function denoted by $A\Psi$.
- The linearity of the operator means that a linear combination of two wave functions Ψ_1 and Ψ_2 is converted into the same linear combination of $A\Psi_1$ and $A\Psi_2$.

$$A(C_1\Psi_1 + C_2\Psi_2) = C_1(A\Psi_1) + C_2(A\Psi_2) \qquad ... (2.5)$$

> The dynamical variables in quantum mechanics do not commute

i.e.
$$AB \neq BA$$

 \triangleright The difference AB-BA is called the commutator of A and B. In notation

$$[A,B] = AB - BA \qquad \dots (2.6)$$

The commutation relations of position and momentum is deduce as follows:

> For one dimension

$$(xp - px)\Psi = \left[x(-i\hbar\vec{\nabla}) - (-i\hbar\vec{\nabla})x\right]\Psi$$

$$= -i\hbar\left[x\frac{\partial}{\partial x}\Psi - \frac{\partial}{\partial x}(x\Psi)\right]$$

$$= -i\hbar\left[x\frac{\partial\Psi}{\partial x} - \frac{\partial x}{\partial x}\Psi - x\frac{\partial\Psi}{\partial x}\right]$$

$$\therefore (xp - px)\Psi = i\hbar\Psi$$

$$\therefore [x, p] = i\hbar \qquad ... (2.7)$$
Insigns

> For three dimensions

dimensions
$$(x_{i}p_{j} - p_{j}x_{i})\Psi = \left[x_{i}\left(-i\hbar\frac{\partial}{\partial x_{j}}\right)\Psi - \left(-i\hbar\frac{\partial}{\partial x_{j}}\right)x_{i}\Psi\right]$$

$$= \left[-i\hbar x_{i}\frac{\partial\Psi}{\partial x_{j}} + i\hbar\frac{\partial}{\partial x_{j}}(x_{i}\Psi)\right]$$

$$= -i\hbar\left[x_{i}\frac{\partial\Psi}{\partial x_{j}} - \frac{\partial x_{i}}{\partial x_{j}}\Psi - x_{i}\frac{\partial\Psi}{\partial x_{j}}\right]$$

$$= i\hbar\delta_{ij}\Psi$$

$$\therefore \left[x_{i}, p_{j}\right] = i\hbar\delta_{ij} \qquad ... (2.8)$$

Where, $\frac{\partial x_i}{\partial x_j} = \delta_{ij}$ is called Kronecker delta function.

$$\delta_{ij} = 1 \quad if \ i = j$$

$$and \qquad \delta_{ij} = 0 \quad if \ i \neq j$$
Also, $\left[x_i, x_j\right] = 0$, $\left[p_i, p_j\right] = 0$... (2.9)

We can write,

$$[x, p_x] = [y, p_y] = [z, p_z] = i\hbar$$
 ... (2.10)

The basic commutation relations and the identities are

$$[AB, C] = A[B, C] + [A, C]B$$
 ... (2.11)

$$[A, BC] = [A, B]C + B[A, C]$$
 ... (2.12)

Where A, B & C are arbitrary operators.

The Adjoint of an Operator and Self Adjointness:

Let us consider the integral

$$\int \Phi^* A \Psi \, d\tau \equiv (\Phi, A \Psi) \qquad ... (2.13)$$

which involves two different functions ϕ and Ψ and reduces to the special case when $\phi = \Psi$.

Definition: If an operator satisfied following condition is called the adjoint of A and denoted by A^{\dagger} (read as A dagger), such that

$$\int \Phi^* A \Psi \ d\tau = \int (A^{\dagger} \Phi)^* \Psi \ d\tau, \quad or \quad (\Phi, A \Psi) = (A^{\dagger} \Phi, \Psi) \qquad \dots (2.14)$$

In means, the value of integral makes no difference whether A acts on Ψ or its adjoint A^{\dagger} acts on the other wave function Φ .

The properties of an adjoint operator are as follows:

• The adjoint operators are additive

$$(A+B)^{\dagger} = A^{\dagger} + B^{\dagger} \qquad \dots (2.15)$$

• If c is a complex number then

$$(cA)^{\dagger} = c^* A^{\dagger} \qquad \dots (2.16)$$

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

Further, since

$$\int \Phi^*(A^{\dagger} \Psi) d\tau = \left[\int (A^{\dagger} \Psi)^* \Phi d\tau \right]^* = \left[\int \Psi^* A \Phi d\tau \right]^* = \int (A^{\dagger} \Phi)^* \Psi d\tau \quad \dots (2.17)$$

We have

$$(A^{\dagger})^{\dagger} = A$$
 ... (2.18)

• For the adjoint of the product of two operators A and B, is given by

$$\int \Phi^* A B \Psi \ d\tau = \int (A^{\dagger} \Phi)^* B \Psi \ d\tau = \int (B^{\dagger} A^{\dagger} \Phi)^* \Psi \ d\tau \qquad \dots (2.19)$$

or

$$(AB)^{\dagger} = B^{\dagger}A^{\dagger} \qquad \dots (2.20)$$

Definition: An operator A is said to be self adjoint if its adjoint is equal to itself

$$A^{\dagger} = A \qquad \dots (2.21)$$

Or

$$\int \Phi^* A \Psi \ d\tau = \int (A \Phi)^* \Psi \ d\tau, \qquad i. e. \ (\Phi, A \Psi) = (A \Phi, \Psi) \qquad \dots (2.22)$$

- The product of two self-adjoint operators is not necessarily self-adjoint.
- If $A^{\dagger} = A$ and $B^{\dagger} = B$, then according to equation (2.16),

$$(AB)^{\dagger} = BA$$
 ... (2.23)

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

$$(AB + BA)$$
 and $i(AB - BA)$... (2.24)

The expectation value of a self-adjoint operator is real

$$\langle A \rangle = \langle A \rangle^*$$

Thus, self-adjoint operators are suitable for representing observable dynamical variables.

• It may be observed that $A^{\dagger}A$ is always self-adjoint. Its expectation value is non-negative in all states.

$$\langle A^{\dagger}A \rangle = \int \Psi^* A^{\dagger} A \Psi \ d\tau = \int (A \Psi)^* (A \Psi) \ d\tau \ge 0 \qquad \dots (2.25)$$

Any operator with this property is called positive property.

• Hence, the absolute square of the function $A\Psi$ is non-negative.

i.e
$$|A\Psi|^2 \neq 0$$

• Now, if $\langle A^{\dagger}A \rangle$ is to vanish, the integrand must vanish identically. Thus,

$$\langle A^{\dagger}A \rangle = 0$$
 implies $A\Psi = 0$... (2.26)

The Eigen Value Problem: Degeneracy

For any operator A, the eigen value equation can be written as

$$A\phi_a = a\phi_a \qquad \dots (2.27)$$

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 eigen function of A belonging to the eigen value 'a'. The set of all eigen values of A is called the eigen value spectrum of A. The spectrum may be continuous, or discrete, or partly continuous and partly discrete.

If there exist only one eigen function corresponds to a given eigen value, then the eigen value is called non-degenerate.

If there are more than one eigen function for a given eigen value then it is called degenerate.

For any degenerate eigen value, there is always an infinite numbers of eigen function.

Now consider,

Multiplying above equations by C_1 and C_2 respectively and adding, we get

$$A(C_1 \phi_a + C_2 \chi_a) = a(C_1 \phi_a + C_2 \chi_a) \qquad ... (2.29)$$

Hence, $(C_1 \Phi_a + C_2 \chi_a)$ is set of eigen function corresponding to a given value of eigen value. This set forms a linear space. This space is called eigen space belonging to the eigen value 'a' of A.

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

$$C_1 \phi_{a1} + C_2 \phi_{a2} + \dots + C_r \phi_{ar}$$
 ... (2.30)

Where, C_1 , C_2 , C_r are the suitable coefficients.

 $\phi_{a1}, \phi_{a2}, \dots \phi_{ar}$ form a set of basis functions which spans the linear space.

There is an infinite number of ways of choosing a basis. But the number 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 eigen value. We say that the eigen value is r- fold degenerate.

Eigen Values and Eigen Functions of Self Adjoint Operators:

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

$$A^{\dagger} = A \qquad \dots (2.31)$$

or

$$\int \Phi^* A \Psi \ d\tau = \int (A^{\dagger} \Phi)^* \Psi \ d\tau \qquad ... (2.32)$$

or

$$(\phi, A\Psi) = (A^{\dagger}\phi, \Psi) \qquad \dots (2.33)$$

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

$$A \varphi_a = a \varphi_a$$
, $A \varphi'_a = a' \varphi'_a$... (2.34)

The self-adjointness condition is

$$\int \Phi^* A \Psi \ d\tau = \int (A \Phi)^* \Psi \ d\tau \qquad \dots (2.35)$$

Substituting $\varphi=\varphi_a$ and $\varPsi=\varphi_a'$ in equation (2.35), we get

$$\int \Phi^* A \, \Phi'_a \, d\tau = \int (A \Phi_a)^* \, \Phi'_a \, d\tau \qquad \dots (2.36)$$

We have eigen equation $A \varphi_a = a \varphi_a$

Now multiplying this equation by ϕ_{α}^* and taking integral, we get

$$\int \Phi_a^* A \, \Phi_a \, d\tau = a \int \Phi_a^* \, \Phi_a \, d\tau \qquad \qquad \dots (2.37)$$

Similarly, we have $A \varphi_a^* = a^* \varphi_a^*$

$$\int \phi_a A \, \phi_a^* \, d\tau = a^* \int \phi_a \, \phi_a^* \, d\tau \qquad \qquad \dots (2.38)$$

But A is self adjoint, hence from equations (2.37) & (2.38), we can write

$$(a - a^*) \int \phi_a^* \, \phi_a \, d\tau = 0$$
 ... (2.39)

But

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

$$\therefore a = a^* \qquad \dots (2.40)$$

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

Now if,

$$\int \Phi_a^* \, \Phi_a \, d\tau = 0,$$
then $a \neq a^*$... (2.41)

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

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

$$\int \Phi_a^* \, \Phi_a' \, d\tau = \delta(a, a') \qquad \qquad \dots (2.42)$$

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

 $\delta(a, a') = 1$ if ϕ_a is normalizable

 $= \infty$ if ϕ_a is non – normalizable

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

$$\delta(a, a') = \delta_{aa'} \qquad \dots (2.43)$$

For an infinite norm of eigen functions, we write

$$\delta(a,a') = \delta(a-a') \tag{2.44}$$

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

Equation (2.43) applies if ' α ' belongs to the discrete part of the eigen value spectrum, and Equation (2.44) in the case of eigen values belonging to the continuum part of the spectrum.

The Dirac Delta Function:

Definition: 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 particular single point and zero for the other points then its integral or area under the curve will be zero.

Now,

$$\int_{-\infty}^{+\infty} \delta(x - x') dx = 1 \qquad ... (2.45)$$

$$\delta(x - x') = 0 , x \neq x'$$

$$x = x'$$
... (2.46)

$$\delta(x - x') = 0 , x \neq x'$$

$$= \infty, x = x'$$
... (2.46)

The Dirac delta function is also defined through the equation

$$\int_{a}^{b} f(x) \, \delta(x - x') \, dx = f(x'), \ a < x' < b \qquad \dots (2.47)$$

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.

$$\delta(x - x') = 0 \text{ for all } x \neq x' \qquad \dots (2.48)$$

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 equation (2.47)

$$\delta(x - x') = \infty \text{ when } x = x' \qquad \dots (2.49)$$

Fig. (2.1) shows the behaviour of Dirac delta function $\delta_{\epsilon}(x-x')$ as $\epsilon \to 0$.

Here,

$$\delta_{\epsilon}(x - x') = (2\pi\epsilon^2)^{-1/2} exp\left[-(x - x')^2/2\epsilon^2\right]$$
 ... (2.50)

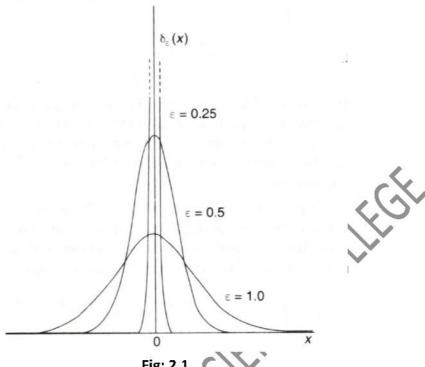


Fig: 2.1

In the $limit \ \epsilon \rightarrow 0$ it satisfied equation (2.49) and also the condition

$$\int \delta (x - x') dx = 1 \qquad \dots (2.51)$$

The three dimensional Dirac delta function is defined by

$$\delta(\vec{X} - \vec{X}') = \delta(x - x') \delta(y - y') \delta(z - z') \qquad \dots (2.52)$$

Observables: Completeness and Normalization of Eigen Functions:

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

Let A be a self-adjoint operator of some physical problem. Its eigen functions $\{\varphi_a\}$ are said to form a complete set if any arbitrary wave function Ψ of the system can be 'expanded' in to linear combination

$$\Psi = \sum C_a \Phi_a + \int C_a \Phi_a \ da \qquad \dots (2.53)$$

The linear combination includes summation over the discrete part of the eigen value spectrum as well as integration over the continuous part. The assumption that a set $\{\varphi_a\}$ 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 eigen value spectrum is discrete, so that second term of equation (2.53) will not be present. Using the orthonormality property of the Φ_a ,

$$\therefore \int \Psi^* \Psi \ d\tau = 1$$

$$\therefore \int \left[\sum_{a'} C_{a'}^* \varphi_{a'}^* \right] \left[\sum_a C_a \varphi_a \right] d\tau = 1$$

$$\therefore \sum_{a'} \sum_a C_{a'}^* C_a \int \varphi_{a'}^* \varphi_a \ d\tau = 1$$

$$\therefore \sum_{a'} \sum_a C_{a'}^* C_a \delta(a', a) = 1$$

$$\therefore \sum_a C_a^* C_a \delta(a, a) = 1$$

$$\therefore \sum_a C_a^* C_a \delta(a, a) = 1$$

$$\therefore \text{ we get a single value.}$$

Because, when a = a', we get a single value.

Now, there are two possibilities corresponding to

$$\delta(a,a) = 1$$
 or ∞

But, $\delta(a,a) = \infty$ must be rejected because it makes the equation (2.54) inconsistent. Hence, we conclude that "the eigen functions belonging to discrete eigen values are normalizable".

Setting
$$\delta(a,a')=\delta_{aa'}$$
 in above equation, we obtain
$$\sum_a |C_a|^2=1 \qquad \qquad \dots (2.55)$$

If we had a continuous instead of a discrete spectrum for 'a', integral would appear in the place of summation in equation (2.54), and it becomes

$$\int C_a da \int C_{a'}^* \delta_{aa'} da' = 1 \qquad \dots (2.56)$$

The integral over a' vanish if $\delta(a, a')$ is Kronecker delta function and hence equation (2.56) would be inconsistent. Hence, we have to take $\delta(a, a')$ as the Dirac delta function. Therefore, "the eigen functions belonging to continuous eigen values are of infinite norm". Equation (2.56) now simplifies to

$$\int |C_a|^2 da = 1 \qquad (2.57)$$

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

$$\sum |C_a|^2 + \int |C_a|^2 da = 1 \qquad ... (2.58)$$

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

$$\Psi = \sum_{a} C_a \phi_a \qquad \dots (2.59)$$

and
$$\int \phi_a^* \, \phi_{a'} \, d\tau = \, \delta_{aa'} \qquad \qquad \dots (2.60)$$

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 closure

$$\sum_{a} \phi_{a}(\vec{X})\phi_{a}^{*}(\vec{X}') = \delta(\vec{X} - \vec{X}') \qquad \dots (2.61)$$

This can be prove as follows:

Let

$$\Psi = \sum_{m} C_m \Phi_m \tag{2.62}$$

Multiplying on both the sides by φ_n^\ast and integrating, we get

$$\int \Phi_n^* \Psi \ d\tau = \sum_m C_m \int \Phi_n^* \Phi_m \ d\tau \qquad \dots (2.63)$$

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

$$\therefore \int \phi_n^* \Psi d\tau = \sum_m C_m \delta_{m,n} = C_n$$

$$\therefore C_n = \int \phi_n^* \Psi d\tau \qquad \dots (2.64)$$

Multiplying on both the sides by
$$\phi_n^*$$
 and integrating, we get
$$\int \phi_n^* \Psi \ d\tau = \sum_m C_m \int \phi_n^* \phi_m \ d\tau \qquad \dots (2.63)$$
 But, $\{\phi_n\}$ are orthonormal to each other. Hence,
$$\phi_n^* \phi_m \ d\tau = \delta_{m,n}$$

$$\therefore \int \phi_n^* \Psi \ d\tau = \sum_m C_m \delta_{m,n} = C_n$$

$$\therefore C_n = \int \phi_n^* \Psi \ d\tau \qquad \dots (2.64)$$
 Substituting equation (2.64) in (2.62), we get
$$\Psi = \sum_m \left[\int \phi_m^* \Psi \ d\tau\right] \phi_m$$

$$= \sum_m \int \left[\phi_m^* (\vec{r}') \Psi (\vec{r}') \ d\tau'\right] \phi_m(\vec{r})$$

$$\Psi(\vec{r}) = \sum_m \int \left[\phi_m^* (\vec{r}') \Psi (\vec{r}') \ d\tau'\right] \Psi(\vec{r}') \ d\tau' \qquad \dots (2.65)$$
 In this equation,
$$\sum_m \phi_m^* (\vec{r}') \ \phi_m(\vec{r}) \ \text{must be } \delta(\vec{r} - \vec{r}')$$

In this equation,

$$\sum_{m} \phi_{m}^{*}(\vec{r}') \phi_{m}(\vec{r}) \text{ must be } \delta(\vec{r} - \vec{r}')$$

$$\Psi(\vec{r}) = \sum_{m} \int \delta(\vec{r} - \vec{r}') \, \Psi(\vec{r}') \, d\tau' \qquad \dots (2.66)$$

$$\sum_{m} \phi_{m}^{*}(\vec{r}) \phi_{m}(\vec{r}') = \delta(\vec{r} - \vec{r}') \text{ is the closure of } \{\phi_{m}\}$$

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

$$\sum_{a} \Phi_{a}(\vec{X}) \Phi_{a}^{*}(\vec{X}') = \delta(\vec{X} - \vec{X}') \qquad \dots (2.67)$$

Physical Interpretation of Eigen Values, Eigen Functions and Expansion Coefficients:

Suppose A is the dynamical operator of any 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,

$$\Psi = \sum_{a} C_a \Phi_a \qquad ... (2.68)$$

Where, C_a is the coefficient.

$$C_a = \int \phi_a^* \, \Psi \, d\tau \tag{2.69}$$

For normalization of Ψ

$$\sum_{\alpha} |C_{\alpha}|^2 = 1 \qquad ... (2.70)$$

Here, we consider Ψ is normalized.

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

The expectation values of dynamical operator A is given by

$$\langle A \rangle = \int \Psi^* A \Psi d\tau$$

$$\therefore \langle A \rangle = \int \left(\sum_{a'} C_{a'}^* \varphi_{a'}^* \right) A \left(\sum_{a} C_a \varphi_a \right) d\tau$$

$$\therefore \langle A \rangle = \sum_{a} \sum_{a'} C_a C_{a'}^* \int \varphi_{a'}^* A \varphi_a d\tau$$

But, $A\phi_a = a\phi_a$

The function ϕ_a are orthonormal. Hence, $\delta_{aa'}=1$ for a=a'. Equation (2.71) states that $\langle A \rangle$ is the weighted average of the eigenvalues 'a' of A. The weight factors are the positive quantities $|\mathcal{C}_a|^2$ whose sum is unity.

The physical meaning of these observations 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 $|\mathcal{C}_a|^2$. 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 $|\mathcal{C}_a|^2$. 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 eigen functions can also be seen.

Suppose Ψ is itself be chosen to be one of the eigen functions of A say $\varphi_{a'}$. In these case

$$C_a = \int \Phi_{a'}^* \, \Phi_a \, d\tau = \, \delta_{aa'} \qquad \dots (2.72)$$

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 eigen functions $\phi_{a'}$ of A represent 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 eigen values of A.

The interpretation of C_a is the probability amplitude and $|C_a|^2$ is a probability density. Hence, if we know the coefficients C_a we can obtain the information about the function Ψ .

Therefore, constraints \mathcal{C}_a as a function of $\$, it is called 'A-state wave function' just as $\Psi(\vec{X})$ is called the 'coordinate space' or 'configuration space wave function'. We say that \mathcal{C}_a and $\Psi(\vec{X})$ are different representation of the state. \mathcal{C}_a is represented by column matrix as,

$$C_a = \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ \vdots \\ \vdots \\ C_n \end{bmatrix}$$

This matrix is called A — representation of the state Ψ .

Momentum Eigen Functions; Wave Functions in Momentum Space:

Eigen value Equation:

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

The eigen value equation is

$$-i\hbar \frac{d\Phi_p}{dx} = p\Phi_p \qquad ... (2.73)$$

Where, p is eigen value and φ_p is corresponding eigen function.

Now in quantum mechanics

$$p = \hbar k \qquad \qquad \dots (2.74)$$

The eigen function corresponding to k is ϕ_k

Hence, equation (2.73) becomes

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

$$\therefore \frac{d\Phi_{k}}{dx} = ik\Phi_{k} \qquad (\text{Here, } i^{2} = -1)$$

$$\therefore \frac{d\Phi_{k}}{\Phi_{k}} = ik \, dx$$

Integrating this relation, we get

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

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

$$\therefore \phi_k = Ce^{ikx} \qquad \dots (2.75)$$

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

Normalization of Momentum Eigen Functions:

From equation (2.75), 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.

$$\therefore \int_{0}^{L} \varphi_{k}^{*}(x)\varphi_{k}(x) dx = C^{2} \int_{0}^{L} e^{-ikx} e^{ikx} dx$$

$$\therefore \int_{0}^{L} \varphi_{k}^{*}(x)\varphi_{k}(x) dx = C^{2} \int_{0}^{L} dx = C^{2}L$$

$$\therefore \int_{0}^{L} \varphi_{k}^{*}(x)\varphi_{k}(x) dx = C^{2}L$$

For normalization it should be 1.

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

Hence, equation (2.75) becomes

$$\Phi_k = \frac{1}{\sqrt{L}} e^{ikx} \qquad \dots (2.76)$$

This is a box normalized momentum eigen functions.

For three dimensional

$$\Phi_{\vec{k}} = \frac{1}{L^{3/2}} e^{i\vec{k}\cdot\vec{r}} \qquad ... (2.77)$$

(b) δ – Function Normalization:

For box-normalization following condition must be satisfied

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

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

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

Hence,

$$k = \frac{2\pi}{L}n \qquad \dots (2.78)$$

Where, $n = \pm 1, \pm 2, ...$

Equation (2.78) represents that the momentum of the particle is discrete. It is not true. In actual practice, the momentum must be continuous. If the eigen values are

continuum then we take δ — function normalization. Hence, we must find a normalization factor in such that

$$\int_{-\infty}^{+\infty} \Phi_{k'}^* \Phi_k \ dx = \delta(k - k') \qquad \dots (2.79)$$

But,

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

$$\lim_{g \to \infty} 2C^2 \left[\frac{\sin(k - k')g}{(k - k')} \right] = \delta(k - k') \qquad \dots (2.80)$$

But,
$$\delta(x) = \lim_{g \to \infty} \frac{\sin gx}{\pi x}$$
 ... (2.81)

In this case

$$\delta(k-k') = \lim_{g\to\infty} \frac{\sin g(k-k')}{\pi (k-k')} \qquad \dots (2.82)$$

Hence, equation (2.80) can be written as

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

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

$$\therefore 2 \pi C^{2} = 1$$

$$\therefore C = \frac{1}{(2\pi)^{1/2}} \qquad \dots (2.83)$$

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

$$\Phi_k = \frac{1}{(2\pi)^{1/2}} e^{ikx} \qquad \dots (2.84)$$

In three dimensions

$$\Phi_{\vec{k}} = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{X}} \qquad ... (2.85)$$

Closure Property of Momentum Eigen Functions:

(a) Box Normalized Eigen Functions:

The closure property is

Hormalized Eigen Functions:
losure property is
$$\sum_{n=-\infty}^{+\infty} \varphi_k^*(x) \varphi_k(x') = \delta(x-x') \qquad ... (2.86)$$
But, $k = \frac{2\pi}{L} n$, and $\varphi_k = \frac{1}{\sqrt{L}} e^{ikx}$

$$\therefore \sum_{n=-\infty}^{+\infty} \varphi_k^*(x) \varphi_k(x') = \sum_{n=-\infty}^{+\infty} \frac{1}{L} e^{-i\frac{2\pi}{L}nx} e^{i\frac{2\pi}{L}nx}$$

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

$$\therefore \sum_{n=-\infty}^{+\infty} \varphi_k^*(x) \varphi_k(x') = \lim_{N\to\infty} \frac{1}{L} \sum_{n=-N}^{+N} e^{-i\frac{2\pi}{L}n(x-x')} \qquad ... (2.87)$$
sical series. Its first component is
$$a = e^{i\frac{2\pi}{L}N(x-x')}$$
of two remaining terms is

This is a physical series. Its first component is

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

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 solution of series

$$S = a + ap + ap^{2} + \cdots + ap^{n-1} = a\frac{1 - p^{n}}{1 - p}$$

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

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

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

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

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

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

$$\therefore \sum_{n = -\infty}^{+\infty} \Phi_k^*(x) \Phi_k(x') = \delta(x - x') \qquad \dots (2.88)$$

(b) δ – Function Normalized Eigen Functions:

We know that

$$\Phi_{k} = \frac{1}{(2\pi)^{1/2}} e^{ikx} \qquad ...(2.89)$$

$$\therefore \sum_{k} \Phi_{k}(x) \, \Phi_{k}^{*}(x') = \sum_{k} \frac{1}{2\pi} e^{ik(x-x')}$$

But, k is continuum, hence above equation becomes

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

In three dimensions

$$\sum_{k'} \phi_{\vec{k}}(\vec{r}) \, \phi_{\vec{k}}^*(\vec{r}') = \delta(\vec{r} - \vec{r}') \qquad \dots (2.91)$$

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

$$: \Psi(\vec{r}) = \sum_{\vec{k}} C(\vec{k}) \, \phi_{\vec{k}}(\vec{r}) \qquad \dots (2.92)$$

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

$$\oint \Phi_{\vec{k}'}^*(\vec{r}) \ \Psi(\vec{r}) \ d^3r = \sum_{\vec{k}} C(\vec{k}) \int \Phi_{\vec{k}'}^* \ \Phi_k \ d^3r$$

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

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

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

$$\therefore C(\vec{k}) = \int \Phi_{\vec{k}'}^*(\vec{r}) \ \Psi(\vec{r}) \ d^3r \qquad \dots (2.93)$$

Now,

$$\phi_{\vec{k}}^*(\vec{r}) = \frac{1}{(2\pi)^{3/2}} e^{-i\vec{k}\cdot\vec{r}}
\therefore C(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \int \Psi(\vec{r}) e^{-i\vec{k}\cdot\vec{r}} d^3r \qquad \dots (2.94)$$

For continuous distribution, equation (2.92) can be written as,

$$\Psi(\vec{r}) = \int C(\vec{k}) \, \phi_{\vec{k}}(\vec{r}) \, d^3r \qquad \dots (2.95)$$

where,

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

$$: \Psi(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \int C(\vec{k}) e^{i\vec{k}\cdot\vec{r}} d^3r \qquad (2.96)$$

Equations (2.94) & (2.95) are Fourier transform to each other.

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

2.95) are Fourier transform to each other.
$$\vec{k} \text{ , then we get}$$

$$\Psi(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}} \int C(\vec{p}) \ e^{i(\vec{p}\cdot\vec{r})/\hbar} \ d^3p \qquad ... (2.97)$$

$$C(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int \Psi(\vec{r}) \ e^{-i(\vec{p}\cdot\vec{r})/\hbar} \ d^3r \qquad ... (2.98)$$
97) shows that if $\Psi(\vec{r})$ represent the state of the system of observable probability to get the momentum \vec{p} is $|C(\vec{p})|^2$. It is given by equation

and
$$C(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int \Psi(\vec{r}) e^{-i(\vec{p}\cdot\vec{r})/\hbar} d^3r$$
 ... (2.98)

Equation (2.97) shows that if $\Psi(\vec{r})$ 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 equation (2.98). $\Psi(\vec{r})$ is the Fourier transform of $C(\vec{k})$.

The expectation value of any function on momentum is

$$\langle f(\vec{p})\rangle = \int |C(\vec{p})|^2 f(\vec{p}) d^3p \qquad \dots (2.99)$$

 $\mathcal{C}(\vec{p})$ 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

$$\vec{X}_{op} = i\hbar \nabla_{\vec{p}} \qquad \dots (2.100)$$

$$\vec{X}_{op} = i\hbar \nabla_{\vec{p}}$$
 ... (2.100)
and $\vec{p}_{op} = \vec{p}$... (2.101)

where,
$$\nabla_p = \left(\frac{\partial}{\partial p_x}, \frac{\partial}{\partial p_y}, \frac{\partial}{\partial p_z}\right)$$

Eigen value equation of position operator in momentum space:

The eigen equation of position operator in momentum space is given by

$$\vec{r}_{op} C(\vec{p}) = \vec{r} C(\vec{p})$$
 ... (2.102)

But,

$$C(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int \Psi(\vec{r}) \ e^{-i(\vec{p}\cdot\vec{r})/\hbar} \ d^3r \qquad ...(2.104)$$

> Example: 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.

$$C(k) = \frac{1}{(2\pi)^{1/2}} \int \Psi(r) e^{-ikx} dx$$

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

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

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

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

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

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

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

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

Question Bank

Mul	ltip	le c	hoi	ce	aues [,]	tions
					9000	

(1)	For the wave functions \emptyset and ψ and operator	r A the shorter notation of the integral
	$\int \phi^* A \psi d\tau \equiv \underline{\hspace{1cm}}$	
	(a) (ϕ, ψ)	(b) $(\phi^*, A\psi)$
	(c) $(\phi, A\psi)$	(d) $(A \phi, \psi)$
(2)	For adjoint operator A, (ϕ , $A\psi$)=	
	(a) $(A^+\emptyset, \psi)$	(b) $(\phi^*, A\psi)$
	(c) $(\phi, A\psi)$	(d) $(A \phi, \psi)$
(3)	For the adjoint of the product of two operato	The state of the s
3 A	(a) B ⁺ A ⁺	(b) AB
	(c) A [†] B [†]	(d) 1
(4)	If there exist only one eigen function correspond	
(-)	eigen value is called	
	(a) Non degenerate	(b) Degenerate
	(c) Discrete	(d) Continuum
(5)	If there exist more than one eigen function co	
(-)	the eigen value is called	STESPONE STONE SIGNATURE, STONE
	(a) Non degenerate	(b) Degenerate
	(c) discrete	(d) Continuum
(6)	The set of eigen function $(C_1 \emptyset_a + C_2 \psi_a)$ for	
(5)	(a) Configuration	(b) eigen
	(c) Phase	(d) Imaginary
(7)	If A is an operator and A [†] is an adjoint operator	
(*)	(a) A	(b) A*
	(c) A [†]	(d) 1
(8)	If A and B are non-commutative self adjoint o	
(0)	(a) BA	(b) AB
	(c) A [†] B [†]	(d) 1
(9)	Eigen values of a self adjoint operator is	(0) 1
(3)	(a) always 0	 (b) Infinite
	(c) Real	(d) Imaginary
(10)	For any operator A and a wave function ϕ_a if	, , , ,
(10)	(a) Eigen function	(b) Eigen value
	(c) Probability density	(d) Probability amplitude
(11)	Any two eigen functions belonging to unequa	304 Maria 20 1000 Maria 200 Maria 20
(++)	are	ar eigen values of a sen adjoint operator
	(a) Non orthogonal	(b) Parallel
	(c) Orthogonal	(d) Imaginary
(12)	If $\delta_{m,n}$ is Kronecker delta function then $\delta_{m,n}$:	, , , , ,
\/	(a) $m=n$	(b) $m > n$
	(c) $m < n$	(d) $m \neq n$
(13)	If $\delta_{m,n}$ is Kronecker delta function then $\delta_{m,n}$:	Section 4. Control of the control of
(44)	(a) $m=n$	(b) $m > n$
	(c) $m - n$	(d) $m \neq n$
(14)	30 PV	
(14)	An operator representing observable dynamic	
	(a) always 0	(b) Infinite

(c) Real

- (d) Imaginary
- (15) Position operator in a momentum space is given by $r_{op} =$
 - (a) iħV_D

(b) $i\hbar r_{op}$

(c) $\left(\frac{\partial}{\partial x}\hat{i} + \frac{\partial}{\partial y}\hat{j} + \frac{\partial}{\partial z}\hat{k}\right)$

- (d) $\frac{2m}{\hbar^2} \vec{\nabla}$
- (16) If A & B are a canonically conjugate pair of operator, then [A, B] =
 - (a) Iħ/2

(b) Iħ

(c) To

- (d) 2iħ
- (17) The value of constant of integration for Box normalized momentum eigen function is
 - (a) $1/(2\sqrt{L})$

(b) $1/\sqrt{L}$

(c) $1/\sqrt{\pi}$

- (d) $1/\sqrt{2\pi}$
- (18) The value of constant of integration for δ function normalized momentum eigen function is
 - (a) $1/(2\sqrt{L})$

(b) $1/\sqrt{l}$

(c) $1/\sqrt{\pi}$

(d) $1/\sqrt{2\pi}$

Short Questions:

- 1. State the postulates of quantum mechanics
- 2. Explain adjoint and self adjoint operator
- 3. Write the properties of an adjoint operator
- 4. Define degenerate and non-degenerate eigen values
- 5. Explain briefly Dirac delta function
- 6. What is observable? Also state expansion postulate
- 7. Show that eigen value of a self adjoint operator is real
- 8. Show that if ϕ_a is eigen function of an operator A and an operator B is commuting with the operator A then ϕ_a is also eigen function of the operator B
- 9. Obtain eigen function in momentum space

Long Questions:

- 1. Discuss the adjoint of operator with their properties
- 2. Discuss the eigen value problem for degeneracy
- 3. Define self adjoint operator and describe its eigen values and eigen functions
- Show that any two eigen functions belonging to distinct (unequal) eigen values of a self adjoint operator are mutually orthogonal
- 5. Show that the eigen function belonging to discrete eigen values are normalizable and the eigen functions belonging to continuous eigen values are of infinite norm.
- 6. Discuss the physical interpretation of eigen values, eigen functions and expansion coefficients
- 7. Write a detailed note on Dirac delta function
- 8. Discuss the completeness and normalization of eigen functions for observables
- 9. Derive eigen function in momentum space and normalized it by box normalization
- 10. Derive eigen function in momentum space and normalized it by δ function normalization method