UNIT-01

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 # Quantum Mechanics :- Branch of physics that explains the behaviour of very small particles like atoms, electron (microscopic particles). It's based on the idea that these particles can act like both particles and waves and it uses complex mathematical equations to predict their behavior with high precision.

> <u>Why Quantum mechanics uses complex mathematics :-</u>
>
> Since microscopic particles act like both waves and particles at the same time. Complex numbers help us understand this by allowing us to work with numbers that have both real and imaginary parts.

Dirac's bra and ket notation :

<u>ket vector</u> :- Each dynamical state may be represented by a certain type of vector known as ket vector or ket represented by symbol $|\psi\rangle$.

$|\psi\rangle$ is represented by column matrix.

$$|\psi\rangle = \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \vdots \\ \phi_n \end{bmatrix} \rightarrow \text{Column Matrix}$$

<u>Bra vector</u> :- Conjugate Transpose matrix of ket vector. Bra vector represented by $\langle\psi|$.

$\langle\psi|$ represents row matrix.

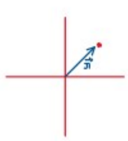
$$\langle\psi| = (|\psi\rangle)^{+} = [\phi_1^* \ \ \phi_2^* \ \ \phi_3^* \ \ \ldots\ldots] \rightarrow \text{Row matrix}$$

Linear vector space :-

→ Also known as vector space and linear space

Types

Real vector space	Complex vector space
for classical systems	for quantum mechanical systems.



$\vec{r} = x\hat{i} + y\hat{j}$

$\vec{r} = (x, y)$

Important : We'll study only complex linear space for quantum mechanics.

Complex linear space / Complex vector space / Complex linear vector space :-

Complex linear space / Complex vector space / Complex linear vector space :-

A vector space $|\psi\rangle = \{|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, ----\}$ in which elements can be multiplied by complex number α or added to one another to give member of same set, is said to form linear vector space $|\psi\rangle$.

The elements of the vector space are vectors

If $|\phi_1\rangle$ and $|\phi_2\rangle$ are in $|\psi\rangle$.

then $\alpha|\phi_1\rangle$ and $|\phi_1\rangle + |\phi_2\rangle$ are also in $|\psi\rangle$.

Mathematical properties of linear vector spaces :-

→ Rules for addition :-

(i) If $|\phi_1\rangle$ and $|\phi_2\rangle$ are elements of vector space then $|\phi_1\rangle$ and $|\phi_2\rangle$ will also be the element of same vector space.

(ii) Commutativity : $|\phi_1\rangle + |\phi_2\rangle = |\phi_2\rangle + |\phi_1\rangle$

(iii) Associativity : $\left(|\phi_1\rangle + |\phi_2\rangle\right) + |\phi_3\rangle = |\phi_1\rangle + \left(|\phi_2\rangle + |\phi_3\rangle\right)$

(iv) Existance of null vector or zero vector :

$$|\phi_1\rangle + |0\rangle = |\phi_1\rangle$$

Here $|0\rangle$ = zero or null vector

(v) Existance of symmetric or inverse vector :

for each vector $|\phi_1\rangle$, there must exist a vector $|-\phi_1\rangle$ such that :

$$|\phi_1\rangle + \underbrace{|-\phi_1\rangle}_{\text{symmetric or inverse vector.}} = |0\rangle = \text{Null vector}$$

→ Rules for multiplication :

(i) Distributive law of Multiplication :

$$(\alpha + \beta)|\phi_1\rangle = \alpha|\phi_1\rangle + \beta|\phi_1\rangle$$

$$\alpha\left(|\phi_1\rangle + |\phi_2\rangle\right) = \alpha|\phi_1\rangle + \alpha|\phi_2\rangle$$

(ii) Associative law of Multiplication :

$$\alpha\beta\left(|\phi_1\rangle\right) = \alpha\left(\beta|\phi_1\rangle\right)$$

(iii) Existance of unit element or null vector :

$$I|\phi_1\rangle = |\phi_1\rangle$$, where I is identity (or unit) operator.

$$0|\phi_1\rangle = |0\rangle \rightarrow \text{null vector.}$$

Linear idependence of vectors and dimensions :-

A linear combination of vectors $|\phi_1\rangle, |\phi_2\rangle, \ldots, |\phi_n\rangle$ is vector $|\phi\rangle$ of the form :-

$$|\phi\rangle = \alpha_1|\phi_1\rangle + \alpha_2|\phi_2\rangle + \ldots + \alpha_n|\phi_n\rangle$$

$$|\phi\rangle = \sum_{i=n}^{n} \alpha_i u_i$$

Where $\alpha_i (i=1,2,3,\ldots n)$ are complex numbers.

The vectors $|\phi_1\rangle, |\phi_2\rangle, \ldots |\phi_n\rangle$ are said to be linearly dependent if :-

$$\alpha_1|\phi_1\rangle + \alpha_2|\phi_2\rangle + \ldots + \alpha_n|\phi_n\rangle = 0$$

$$\sum_{i=n}^{n} \alpha_i u_i = 0 \quad (\text{with } \alpha_i \neq 0 \text{ for } i=1,2,3,\ldots n) \text{ ——— } (1)$$

On the other hand, if there exists no relation exist like equation (1) unless $\alpha_i = 0$ for all value of $i = 1,2,3,\ldots n$, then the vectors $|\phi_1\rangle, |\phi_2\rangle, \ldots |\phi_n\rangle$ said to be linearly independent.

Basis and Expansion Theorem :-

→ **Basis** :- In n-dimensional space (Linear vector space), we may choose number of sets, each set containing n-vectors $(|\phi_1\rangle, |\phi_2\rangle, \ldots)$ such that the vectors of each set are linearly independent. Any set of n such vectors in n-dimensional (L_n) space is said to form a set of basis vectors or to provide a basis (cor-dinate system in L_n)

→ **Expansion Theorem** :-

If the vectors $|\phi_1\rangle, |\phi_2\rangle, \ldots |\phi_n\rangle$ form a basis in L_n, then any vector $\vec{\alpha}$ in L_n may be expressed as a linear combination of vectors.

$$\vec{\alpha} = \alpha_1|\phi_1\rangle + \alpha_2|\phi_2\rangle + \ldots + \alpha_n|\phi_n\rangle$$

$$\vec{\alpha} = \sum_{i=1}^{n} \alpha_i |\phi_i\rangle$$

This theorem is generally said to be the expansion theorem and the coefficients α_i in the linear combination are called co-ordinates of $\vec{\alpha}$

→ Proof of Expansion Theorem :-

Let $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, ----, |\phi_n\rangle$ be linearly independent vectors which span the n-dimensional space. Let $\vec{\alpha}$ be any vector in this space. Then (n+1) vectors must be linearly dependent. Hence there exists non zero scalers such that

$$a\vec{\alpha} + a_1|\phi_1\rangle + a_2|\phi_2\rangle + ----+ a_n|\phi_n\rangle = 0$$

from above equation, we may solve for $\vec{\alpha}$

$$\vec{\alpha} = -\frac{1}{a}\left(a_1|\phi_1\rangle + a_2|\phi_2\rangle + ----+ a_n|\phi_n\rangle\right) = \sum_{i=1}^{n} \frac{a_i}{a}|\phi_i\rangle$$

Substituting α_i for $-\frac{a_i}{a}$, we get

$$\boxed{\vec{\alpha} = \sum_{i=1}^{n} \alpha_i|\phi_i\rangle}$$ Hence Proved.

Orthonormal Sets :-

If the inner product of two state vectors is zero, then the state vectors are said to be orthogonal to each othe

$$\boxed{\langle\phi|\psi\rangle = 0}$$

If the inner product of state vector with itself is unity, the state vector is said to be normalised to unity.

$$\boxed{\langle\phi|\phi\rangle = 1}$$

$$\boxed{\langle\psi|\psi\rangle = 1}$$

As set of vectors which is orthogonal to all the remaining vectors of the set is called an orthogonal set. If each of the vectors of the set is further normalized to unity, it is called orthonormal set.

Dynamical variables as operator :-

Dynamical variables like energy, momentum, position etc. are called observables. Each observable has a definite operator associated with it.

An operator may be defined as a mathematical term which is used in operation on a function such that it is transferred into another function.

Thus if $\hat{A}$ is an operator applied to a function $u(x)$, then it is changed into a function $v(x)$;

$$\boxed{\hat{A}\, u(x) = v(x)}$$

Examples; Addition, Multiplication, Subtraction, Division, differentiation, gradient etc.

→ Linear Operator :-

In quantum mechanics, we deal with linear operators and even if the term operator is used, it means linear operator only.

An $\hat{A}$ is said to be linear, if it satisfies the following two conditions :

(a) $\hat{A}\left[|\phi_1\rangle + |\phi_2\rangle\right] = \hat{A}|\phi_1\rangle + \hat{A}|\phi_2\rangle$

(b) $\hat{A}\left[c\,|\phi_1\rangle\right] = c\left[\hat{A}|\phi_1\rangle\right]$ Here, c is constant value.

Properties of linear operator :-

(a) Identity operator $(\hat{I})$: The identity operator $(\hat{I})$ is an operator, which operating on a function, leaves the function unchanged.

$$\boxed{\hat{I}|\phi\rangle = |\phi\rangle}$$

(b) Null (or zero) Operator $(\hat{0})$: The null operator is an operator, which operating on a function annihilates the function. Thus if

$$\boxed{\hat{0}|\phi\rangle = 0}$$

Eigenvalues and Eigenfunctions :-

If ψ is well behaved function, then an operator $\hat{P}$ may operate on ψ into two different ways depending on the nature of function ψ :

(i) The operator $\hat{P}$ operating on the function ψ may change the function into another f^n ϕ,

$$\boxed{\hat{P}\psi = \phi} \quad \text{—— (1)}$$

we can't determine exact value of observable

we can determine expected value of observable

(ii) The operator $\hat{P}$, operating on some function ψ, may leave the function unchanged but with a complex or real constant.

$$\boxed{\hat{P}\psi = \lambda\psi} \quad \text{——— (2)}$$

we can determine exact value of observable in this case.

where λ may be real or complex number. In this case the function ψ is a member of the class of physically meaningful function, called the eigen function of the operator $\hat{P}$. The number λ is called the eigenvalue of the operator $\hat{P}$ associated with eigenfunction ψ. Equation (2) is called eigenvalue equation.

Example: Find the value of the constant B that makes e^{-ax^2} an eigenfunction of the operator $\left\{\frac{d^2}{dx^2} - Bx^2\right\}$. What is the corresponding eigenvalue.

Solution:- The eigenvalue equation of operator $\hat{P}$ is :-

$$\hat{P}\psi = \lambda\psi$$

where λ is eigenvalue of the state ψ

Here, $\hat{P} = \frac{d^2}{dx^2} - Bx^2$

$$\psi = e^{-ax^2}$$

$$\hat{P}\psi = \left[\frac{d^2}{dx^2} - Bx^2\right] e^{-ax^2}$$

$$= \frac{d^2}{dx^2}\left(e^{-ax^2}\right) - Bx^2 e^{-ax^2}$$

$$= -2a e^{-ax^2}\left[1 - 2ax^2\right] - Bx^2 e^{-ax^2}$$

$$= \left\{4a^2x^2 - 2a - Bx^2\right\} e^{-ax^2}$$

$$= \left\{(4a^2 - B)x^2 - 2a\right\} e^{-ax^2} \quad \text{——— (1)}$$

If the constant B makes $\psi = e^{-ax^2}$ on R.H.S. must be independent of x, so we have :

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

$$\boxed{B = 4a^2}$$

The equation (1) takes the form :

$$\hat{P}\psi = -2a\, e^{-ax^2}$$

$$\hat{P}\psi = -2a\psi \qquad \text{Hence} \Rightarrow \boxed{\lambda = -2a}$$

eigenvalue.

Postulates of Quantum Mechanics :-

(i) State of quantum mechanical System : The first postulate states that "there is a state vector (or wavefunction) associated with every physical state of the system which contains the entire description."

(ii) Observables and operators : For every physical observable (i.e. classical dynamical variable), there is corresponding linear Hermitian Operator.

(iii) Measurment of Eigenvalues : According to this postulate, the measurment of observable A in state $|\psi\rangle$ is represented by the action of corresponding operator $\hat{A}$ on the state $|\psi\rangle$ and the possible result of such a measurment is only one of the eigenvalues 'a_n' of the corresponding operator.

$$\boxed{\hat{A}\,|\phi_n\rangle = a_n\,|\phi_n\rangle}$$

(iv) Expectation value of measurment : The fourth postulate gives the rules for extracting information from the wave-function. The expectation value of a variable of a system in state ψ is given by :-

$$\boxed{\langle A\rangle = \frac{\int \psi^* \hat{A}\,\psi\,dx}{\int \psi^*\psi\,dx} = \frac{\langle\psi|\hat{A}|\psi\rangle}{\langle\psi|\psi\rangle}}$$

Hermitian Operators :-

If ψ and ψ^* is acceptable normalised wave functions, defined over certain range of configuration space τ, then operator $\hat{P}$ associated with a dynamical variable is Hermitian if

$$\boxed{\int \psi^* \hat{P}\,\psi\,d\tau = \int \hat{P}^*\,\psi^*\psi\,d\tau}$$

In other words, if operator $\hat{P}$ satisfies above equation, whenever ψ^* and ψ are normalised, Hermitian, self-adjoint or real operator.

Properties of Hermitian Operator :-

Theorem-01 :- Hermitian operators have real eigenvalues.

Proof: Let λ be an eigenvalue of Hermitian operator in the state described by normalised wavefunction ψ.

Then eigenvalue equation is

$$\hat{P}\psi = \lambda\psi \quad \text{—— (1)}$$

Taking its complex conjugate

$$\hat{P}^*\psi^* = \lambda^*\psi^* \quad \text{—— (2)}$$

According to condition of Hermitian operator:

$$\int \psi^* \hat{P}\psi \, d\tau = \int \hat{P}\psi^* \psi \, d\tau \quad \text{—— (3)}$$

Using equation (1), (2) and (3) gives:

$$\int \psi^* \lambda \psi \, d\tau = \int \lambda^* \psi^* \psi \, d\tau$$

$$\lambda \int \psi^* \psi \, d\tau = \lambda^* \int \psi^* \psi \, d\tau$$

$$(\lambda - \lambda^*) \int \psi^* \psi \, d\tau = 0$$

$\because \int \psi^* \psi \, d\tau = 1$ (condition of normalisation)

$$\lambda - \lambda^* = 0$$

$$\boxed{\lambda = \lambda^*}$$

This is only possible if λ is real number.

This proves that, the eigenvalue of each Hermitian operator is real.

Theorem-02: Two eigen functions of Hermitian operators, belonging to different eigenvalues, are orthogonal.

Proof:

Let $\hat{P}$ be any Hermitian operator and ψ_1 and ψ_2 be two eigen functions of operator $\hat{P}$.

If λ_1 and λ_2 are distinct eigenvalues of operator $\hat{P}$ corresponding to eigenfunctions ψ_1 and ψ_2 then eigenvalue equations are :-

$$\left.\begin{aligned} \hat{P}\psi_1 &= \lambda_1 \psi_1 \\ \hat{P}\psi_2 &= \lambda_2 \psi_2 \end{aligned}\right\} \quad \text{—— (1)}$$

Complex conjugates of these equations are :

$$\hat{P}^*\psi_1^* = \lambda_1^*\psi_1^* \quad \text{or} \quad \hat{P}^*\psi_1^* = \lambda_1\psi_1^*$$

complex conjugates of these equations are:

$$\left.\begin{aligned} \hat{P}^*\psi_1^* &= \alpha_1^*\psi_1^* \quad \text{or} \quad \hat{P}^*\psi_1^* = \alpha_1\psi_1^* \\ \hat{P}^*\psi_2^* &= \alpha_2^*\psi_2^* \quad \text{or} \quad \hat{P}^*\psi_2^* = \alpha_2\psi_2^* \end{aligned}\right\} \quad \text{(2)}$$

According to general conditions of Hermitian operator $\hat{P}$, we have

$$\int \psi_2^*\hat{P}\psi_1\, d\tau = \int \hat{P}^*\psi_2^*\psi\, d\tau$$

Using (1) and (2) we get :-

$$\int \psi_2^*\alpha_1\psi_1\, d\tau = \int \alpha_2\psi_2^*\psi_1\, d\tau$$

$$\alpha_1\int \psi_2^*\psi_1\, d\tau = \alpha_2\int \psi_2^*\psi_1\, d\tau$$

$$(\alpha_1-\alpha_2)\int \psi_2^*\psi_1\, d\tau = 0$$

As $\alpha_1 \neq \alpha_2$, we have $\int \psi_2^*\psi_1\, d\tau = 0$

Thereby indicating that ψ_1 and ψ_2 are orthogonal functions.

Theorem-03: If two Hermitian operator commute, then their product is also Hermitian operator.

Proof. Let ψ_1 and ψ_2 be two functions and $\hat{A}$ and $\hat{B}$ be two Hermitian operators.

Now, consider the integral

$$\int \psi_1^*\hat{A}\hat{B}\psi_2\, d\tau$$

If $\hat{A}$ is Hermitian operator, then

$$\int \psi_1^*\hat{A}\hat{B}\psi_2\, d\tau = \int \psi_1^*\hat{A}(\hat{B}\psi_2)\, d\tau$$

$$= \int \hat{A}^*\psi_1^*(\hat{B}\psi_2)\, d\tau \quad \text{(1)}$$

Again $\hat{B}$ is Hermitian operator, we have :-

$$\int (\hat{A}^*\psi_1^*)\hat{B}\psi_2\, d\tau = \int \hat{B}^*\hat{A}^*\psi_1^*\psi_2\, d\tau \quad \text{(2)}$$

From eq^n (1) and (2), we have

$$\int \psi^*\hat{A}\hat{B}\psi_2\, d\tau = \int \hat{B}^*\hat{A}^*\psi_1^*\psi_2\, d\tau \quad \text{(3)}$$

If operators $\hat{A}$ and $\hat{B}$ commute, we have :-

$$\hat{A}\hat{B} = \hat{B}\hat{A} \quad \text{or} \quad \hat{A}^*\hat{B}^* = \hat{B}^*\hat{A}^*$$

In view of this, equation ③ becomes :-

$$\int \psi_1^* \hat{A}\hat{B}\psi_2 \, d\tau = \int \hat{A}^*\hat{B}^* \psi_1^*\psi_2 \, d\tau$$

Which is the condition for the operator $(\hat{A}\hat{B})$ to be Hermitian operator.

Hence if $\hat{A}$ and $\hat{B}$ are commutating Hermitian operators, then their product operator $\hat{A}\hat{B}$ is also Hermitian operator.

Ques: Show that the momentum operator $\frac{\hbar}{i}\frac{\partial}{\partial x}$ is Hermitian.

$$\int \psi^* \hat{p}\, \psi \, d\tau = \int \hat{p}^* \psi^* \psi \, d\tau$$

Solⁿ :

Momentum operator : $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$ and $\hat{p}^* = -\frac{\hbar}{i}\frac{\partial}{\partial x}$

If $\hat{p}$ is hermitian operator, its expectation value $\langle p \rangle$ in any state ψ must be real.

i.e. $$\langle \hat{p} \rangle = \int_{-\infty}^{+\infty} \psi^* \frac{\hbar}{i}\frac{\partial \psi}{\partial x} \, dx \qquad \text{——— ①}$$

must be real

Integrating eqⁿ ①, we get

$$\langle \hat{p} \rangle = \frac{\hbar}{i}\left[\psi^*\psi\right]_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} \frac{\hbar}{i}\frac{\partial \psi^*}{\partial x}\psi \, dx$$

$$\langle \hat{p} \rangle = \int_{-\infty}^{+\infty} \psi \left[\frac{\hbar}{i}\frac{\partial \psi}{\partial x}\right]^* dx = \langle \hat{p} \rangle^* \qquad \text{——— ②}$$

From eqⁿ ① and ②, we can say that $\langle \hat{p} \rangle$ is equal to its complex conjugate. In other words $\langle p \rangle$ is real. Hence we may say that momentum operator $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$ is Hermitian.

Matrix representation of operators :-

If $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, \ldots\ldots |\phi_n\rangle$ are the eigen states of an operator $\hat{A}$, then matrix form of operator $\hat{A}$ will be a square matrix of order $n \times n$, which can be written as:

$$\hat{A} = \begin{bmatrix} A_{11} & A_{12} & \cdots\cdots & A_{1n} \\ A_{21} & A_{22} & \cdots\cdots & A_{2n} \\ A_{31} & A_{32} & \cdots\cdots & A_{3n} \\ \vdots & \vdots & & \\ A_{n1} & A_{n2} & \cdots\cdots & A_{nn} \end{bmatrix}_{n \times n} = \left[A_{ij}\right]_{n \times n}$$

where elements of matrix A can be calculated by following method :-

$$A_{ij} = \langle \phi_i | \hat{A} | \phi_j \rangle$$

where $i = 1, 2, 3, \ldots n$
$j = 1, 2, 3, \ldots n$

Commutative Operators :-

The commutator of two operators $\hat{A}$ and $\hat{B}$ denoted by $[\hat{A}, \hat{B}]$ is defined as :-

$$\boxed{[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}}$$

→ If $[\hat{A}, \hat{B}] = 0$, then the operators $\hat{A}$ and $\hat{B}$ are said to commute with each other.

$$\hat{A}\hat{B} - \hat{B}\hat{A} = 0$$

$$\boxed{\hat{A}\hat{B} = \hat{B}\hat{A}}$$

→ If $[\hat{A}, \hat{B}] \neq 0$, then the operators $\hat{A}$ and $\hat{B}$ do not commute with each other

$$\boxed{\hat{A}\hat{B} \neq \hat{B}\hat{A}}$$

Properties of Commutators :-

Property - 01 : Antisymmetry property

$$\boxed{[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]}$$

Proof :

By definition we have

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

$$[\hat{A}, \hat{B}] = -\left(\hat{B}\hat{A} - \hat{A}\hat{B}\right)$$

$$\boxed{[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]}$$ Proved

Property - 02 :- Linearity Property

$$\boxed{[\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]}$$

Proof :-

By definition of commutator, we have

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By definition of commutator, we have

$$[\hat{A}, \hat{B}+\hat{C}] = \hat{A}(\hat{B}+\hat{C}) - (\hat{B}+\hat{C})\hat{A}$$

$$= \hat{A}\hat{B} + \hat{A}\hat{C} - \hat{B}\hat{A} - \hat{C}\hat{A}$$

$$= (\hat{A}\hat{B} - \hat{B}\hat{A}) + (\hat{A}\hat{C} - \hat{C}\hat{A})$$

$$\boxed{[\hat{A}, \hat{B}+\hat{C}] = [\hat{A},\hat{B}] + [\hat{A},\hat{C}]}$$ Proved

Property - 03 : Distributive Property

$$\boxed{\begin{aligned} &(a)\ [\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A},\hat{C}] \\ &(b)\ [\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B},\hat{C}] + [\hat{A},\hat{C}]\hat{B} \end{aligned}}$$

Proof (a) :- By definition of commutators we have,

$$[\hat{A}, \hat{B}\hat{C}] = \hat{A}(\hat{B}\hat{C}) - (\hat{B}\hat{C})\hat{A}$$

Adding and subtracting $\hat{B}\hat{A}\hat{C}$ on R.H.S. , we get :

$$[\hat{A},\hat{B}\hat{C}] = \hat{A}\hat{B}\hat{C} - \hat{B}\hat{A}\hat{C} + \hat{B}\hat{A}\hat{C} - \hat{B}\hat{C}\hat{A}$$

$$= (\hat{A}\hat{B} - \hat{B}\hat{A})\hat{C} + \hat{B}(\hat{A}\hat{C} - \hat{C}\hat{A})$$

$$\boxed{[\hat{A},\hat{B}\hat{C}] = [\hat{A},\hat{B}]\hat{C} + \hat{B}[A,\hat{C}]}$$ Proved

Proof (b) :

By definition of commutators we have,

$$[\hat{A}\hat{B}, \hat{C}] = (\hat{A}\hat{B})\hat{C} - \hat{C}(\hat{A}\hat{B})$$

Adding and subtracting $\hat{A}\hat{C}\hat{B}$ on R.H.S. , we get :

$$[\hat{A}\hat{B},\hat{C}] = \hat{A}\hat{B}\hat{C} - \hat{A}\hat{C}\hat{B} + \hat{A}\hat{C}\hat{B} - \hat{C}\hat{A}\hat{B}$$

$$= \hat{A}(\hat{B}\hat{C} - \hat{A}\hat{C}) + \hat{B}(\hat{A}\hat{C} - \hat{C}\hat{A})$$

$$\boxed{[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B},\hat{C}] + \hat{B}[\hat{A},\hat{C}]}$$ Proved

Property - 04 :- Jacobi Identity

Property-04 :- Jacobi Identity

$$\boxed{[\hat{A},[\hat{B},\hat{C}]] + [\hat{B},[\hat{C},\hat{A}]] + [\hat{C},[\hat{A},\hat{B}]] = 0}$$

Proof:

By definition of commutators, we have :-

$$[\hat{A},[\hat{B}\hat{C}]] = \hat{A}[\hat{B},\hat{C}] - [\hat{B},\hat{C}]\hat{A}$$

$$= \hat{A}(\hat{B}\hat{C} - \hat{C}\hat{B}) - (\hat{B}\hat{C} - \hat{C}\hat{B})\hat{A}$$

$$[\hat{A},[\hat{B},\hat{C}]] = \hat{A}\hat{B}\hat{C} - \hat{A}\hat{C}\hat{B} - \hat{B}\hat{C}\hat{A} + \hat{C}\hat{B}\hat{A} \quad \text{——— (1)}$$

Similarly,

$$[\hat{B},[\hat{C},\hat{A}]] = \hat{B}\hat{C}\hat{A} - \hat{B}\hat{A}\hat{C} - \hat{C}\hat{A}\hat{B} + \hat{A}\hat{C}\hat{B} \quad \text{——— (2)}$$

$$[\hat{C},[\hat{A},\hat{B}]] = \hat{C}\hat{A}\hat{B} - \hat{C}\hat{B}\hat{A} - \hat{A}\hat{B}\hat{C} + \hat{B}\hat{A}\hat{C} \quad \text{——— (3)}$$

Adding eqⁿ (1), (2) and (3) we get :-

$$\boxed{[\hat{A},[\hat{B},\hat{C}]] + [\hat{B},[\hat{C},\hat{A}]] + [\hat{C},[\hat{A},\hat{B}]] = 0}$$ Proved

Property-05 :- Any operator always commutes with itself. $[\hat{A},\hat{A}] = 0$

$$\boxed{[\hat{A},\hat{A}] = 0}$$

Proof:

$$\boxed{[\hat{A},\hat{A}] = \hat{A}\hat{A} - \hat{A}\hat{A} = 0}$$ Proved

$[\hat{p},\hat{p}^n] = 0$

Property-06 : Any operator commutes with its own power.

$$\boxed{[\hat{A},\hat{A}^n] = 0 = [\hat{A}^n,\hat{A}]}$$ where $n = 1, 2, 3 \ldots$

Property-07: If λ is constant, than :

$$\boxed{\begin{aligned}[\lambda\hat{A},\hat{B}] &= \lambda[\hat{A},\hat{B}] \\ [\hat{A},\lambda\hat{B}] &= \lambda[\hat{A},\hat{B}]\end{aligned}}$$

EHRENFEST'S THEOREM :-

It states that, the Schrodinger equation leads to the classical (Newton's) laws of motion on the average.

In other words, this theorem states that the average motion of a wave packet agrees with the motion of the corresponding classical particle.

$$\boxed{\frac{d\langle\hat{x}\rangle}{dt} = \frac{\langle\hat{p}\rangle}{m}} \qquad \boxed{\frac{d\langle\hat{p}\rangle}{dt} = \langle -\nabla V\rangle}$$

Proof:

x- component of velocity may be defined as the time rate of change of expactation of x component of position since $\langle x\rangle$ depends upon time

i.e.

$$\frac{d}{dt}\langle x\rangle = \frac{d}{dt}\int_{-\infty}^{+\infty}\psi^*\hat{x}\psi\,d\tau$$

$$= \int_{-\infty}^{+\infty}\psi^* x\frac{\partial\psi}{\partial t}\,d\tau + \int_{-\infty}^{+\infty}\frac{\partial\psi^*}{\partial t}x\psi\,d\tau \qquad \text{——— (1)}$$

Time dependent schrodinger equation :

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

$$\frac{\partial\psi}{\partial t} = \frac{1}{i\hbar}\left\{-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi\right\} \qquad \text{——— (2)}$$

Complex conjugate of time dependent schrodinger equation.

$$-i\hbar\frac{\partial\psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^* + V\psi^*$$

$$\frac{\partial\psi^*}{\partial t} = \frac{1}{-i\hbar}\left\{\frac{-\hbar^2}{2m}\nabla^2\psi^* + V\psi^*\right\} \qquad \text{——— (3)}$$

Using eq^n (2) and (3) in equation (1)

$$\frac{d\langle x\rangle}{dx} = \int_{-\infty}^{+\infty}\psi^* x\left\{\frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi\right)\right\}d\tau + \int_{-\infty}^{+\infty}\left\{\frac{1}{-i\hbar}\left(-\frac{\hbar^2}{2m}\nabla^2\psi^* + V\psi^*\right)\right\}x\psi\,d\tau$$

$$= \frac{1}{i\hbar}\int_{-\infty}^{+\infty}\left[\psi^* x\left[\frac{-\hbar^2}{2m}\nabla^2\psi\right] + \cancel{\psi^* x V\psi} + \frac{\hbar^2}{2m}\nabla^2\psi^* x\psi - \cancel{V\psi^* x\psi}\right]d\tau$$

$$= \frac{-1}{i\hbar}\cdot\frac{\hbar^2}{2m}\int^{+\infty}\left[\psi^* x(\nabla^2\psi) - (\nabla^2\psi^*)x\psi\right]d\tau$$

$$= \frac{-1}{i\hbar} \cdot \frac{\hbar^2}{2m} \int_{-\infty}^{+\infty} \left[\psi^* x (\nabla^2 \psi) - (\nabla^2 \psi^*) x \psi\right] d\tau$$

$$= \frac{-\hbar}{2im} \int_{-\infty}^{+\infty} \psi^* x (\nabla^2 \psi)\, d\tau + \frac{\hbar}{2im} \underbrace{\int_{-\infty}^{+\infty} (\nabla^2 \psi^*) x \psi \, d\tau}$$

Since,

$$\int_{-\infty}^{+\infty} (\nabla^2 \psi^*) x \psi \, d\psi = \int_{-\infty}^{+\infty} \psi^* \nabla^2 (x\psi)\, d\tau$$

$$= \frac{-\hbar}{2im} \int_{-\infty}^{+\infty} \psi^* x (\nabla^2 \psi)\, d\tau + \frac{\hbar}{2im} \int_{-\infty}^{+\infty} \psi^* \nabla^2 (x\psi)\, d\tau$$

$$= \frac{-\hbar}{2im} \int_{-\infty}^{+\infty} \psi^* \left[x(\nabla^2 \psi) - \nabla^2 (x\psi)\right] d\tau$$

Propery :

$$\left[x(\nabla^2 \psi) - \nabla^2 (x\psi)\right] = -2 \frac{\partial \psi}{\partial x}$$

$$\frac{d\langle x \rangle}{dt} = \frac{\hbar}{im} \int_{-\infty}^{+\infty} \psi^* \frac{\partial \psi}{\partial x}\, d\tau$$

$$\frac{d\langle x \rangle}{dt} = \frac{1}{m} \int_{-\infty}^{+\infty} \psi^* \left[\frac{\hbar}{i} \frac{\partial}{\partial x}\right] \psi \, d\tau$$

$$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

$$\frac{d\langle x \rangle}{dt} = \frac{1}{m} \int_{-\infty}^{+\infty} \psi^* \hat{p} \psi \, d\tau$$

$$\langle \hat{p} \rangle = \int_{-\infty}^{\infty} \psi^* \hat{p} \psi \, d\tau$$

$$\boxed{\frac{d\langle x \rangle}{dt} = \frac{\langle \hat{p} \rangle}{m}}$$

Proved