

Chapter-2

M.Sc.

Type of operators

Following are the important type of operators.

1. Linear operators. An operator is said to be linear if it operated on the sum of two or more functions and give the result as sum of the results of operation on each function.

e.g. if A is applied on the sum of two functions $\Psi(x)$ and $\Phi(x)$, linear operator gives

$$\text{Ex: } \frac{\partial}{\partial}(x^3) = 3x^2$$

$$\text{Ex: } \hat{A} \left[\frac{\partial^2}{\partial^2} + 2 \frac{\partial}{\partial} + 3 \right] \text{ the } \hat{A}(x^3) = \frac{\partial^2}{\partial^2}(x^3) + 2 \frac{\partial}{\partial} x^3 + 3x^3 \\ = 6x + 6x^2 + 3x^3$$

$$A [\Psi(x) + \Phi(x)] \neq \sqrt{\Psi(x)} + \sqrt{\Phi(x)}$$

Similarly operator which squares the function or raise the power by three or any number is not linear. But differential operator is linear.

$$\text{i.e. } [\Psi(x) + \Phi(x)] =$$

2. Eigen operators. An operator say A is said to be an Eigen operator if it operator if it operator on a function say

$\Psi(x)$ giving a which is the original function multiplied by some constant.

Following quality should exit.

$$A \Psi(x) = \alpha \Psi(x)$$

$$\text{Ex: } H \Psi = E \Psi$$

$$\text{Ex: } e^{ax} \text{ is a eigen function of } \frac{\partial}{\partial}, \frac{\partial^2}{\partial^2}, \frac{\partial^n}{\partial^n}$$

$$\frac{\partial^n}{\partial^n}(e^{ax}) = a^n e^{ax} \text{ } a^n \text{ is eigen value,}$$

Addition of operator & Subtraction :- $(\hat{A} + \hat{B}) f(x) = \hat{A}f(x) + \hat{B}f(x)$

$$(\hat{A} + \hat{B})f = \hat{A}(F) + \hat{B}(F)$$

$$\text{Ex: } \left[\frac{\partial^2}{\partial^2} + \frac{\partial^2}{\partial^2} \right] F(x,y) = \frac{\partial^2}{\partial^2} F(x,y) + \frac{\partial^2}{\partial^2} F(x,y)$$

Subtraction of operator

$$(\hat{A} - \hat{B})f(x) = \hat{A}f(x) - \hat{B}f(x)$$

$$\text{Ex: } \hat{A} \text{ be } \log_e \text{ \& } \hat{B} \text{ be } \frac{d}{dx} \text{ and } f(x) \text{ be } x^2 \text{ then.}$$

Multiplication of operator :

$$\hat{A}\hat{B} f(x) = \hat{A}(\hat{B}f(x)) = \hat{A}(f''(x))$$

Using operator from righty to left .

$$\text{Ex: } A^2 f(x) \neq [\hat{A} f(x)]^2$$

$$\frac{\partial^2}{\partial^2}(5x^2 + 3x) \frac{\partial}{\partial} \left\{ \frac{\partial}{\partial}(5x^2 + 3x) \right\} = \frac{\partial}{\partial}(10x + 3) = 10.$$

$$[\hat{A} \psi(x)]^2 \left\{ \frac{\partial}{\partial} (5x^2 + 3x) \right\}^2 = 100x^2 + 9 + 60x$$

The constant 'a' is called Eigen value and function $\Psi(x)$ is called Eigen function or *characteristic function* or *proper function of the operator A*.

For example, when an operator $\frac{d^2}{dx^2}$ is carried out on function $\cos 2x$.

$$-\frac{d^2}{dx^2} (\cos 2x) = 4 (\cos 2x)$$

In this case $\cos 2x$ is the eigen function and 4 is **Eigen value** of the operator $\frac{d^2}{dx^2}$.

3. Hermitian operator. If \hat{A} an Eigen operator is on the functions $\Psi_1(x)$ and $\Psi_2(x)$ then it is said to be Hermitian if the following equation holds valid.

$$\int \Psi_2^* \hat{A} (\Psi) d\tau = \int \Psi \hat{A}^* (\Psi_2^*) d\tau$$

Hermitian operator always yields real eigen value. As shown below. If $\Psi_1 = \Psi_2 = \Psi$ the condition for Hermitian nature is $\int \Psi^* \hat{A} (\Psi) d\tau$

Let 'a' be the eigen value of the operator \hat{A} for the eigen function Ψ

$$\therefore \hat{A} \Psi = a \Psi$$

Multiplying both sides by Ψ^* and integrate

$$\int \Psi^* \hat{A} (\Psi) d\tau = \int \Psi^* a \Psi d\tau = a \int \Psi^* \Psi d\tau$$

Taking complex conjugate of each in eigen value equation

$$\hat{A}^* \Psi^* = a^* \Psi^*$$

Multiplying both sides by Ψ and integrating

$$\int \Psi^* \hat{A} (\Psi) d\tau = \int \Psi^* a \Psi d\tau = a^* \int \Psi \Psi^* d\tau$$

Because of Hermitian nature L.H.S of (A) and (B) are equal. Therefore, R.H.S of (A) and (B) are also equal.

$$\therefore a \int \Psi \Psi^* d\tau = a^* \int \Psi \Psi^* d\tau \text{ or } a = a^*$$

Which is true when the constant a, the eigen value of the Hermitian operator is a real number because only real number equal their complex conjugate. It may be noted that for allowed eigen function. The eigen values are always real and the corresponding linear eigen Hermitian operator represents and observable.

Note. All quantum mechanical operator must be linear and hermitian in the nature.

4. Unitary operator. An eigen operator is said to be unitary operator, \hat{a} if it operates on eigen function Ψ_1 and Ψ_2 such that

$$\int \Psi^* (\hat{a}^{-1} \Psi) d\tau = \int \Psi_1 (\hat{a}^{-1} \Psi^*) d\tau$$

Where \hat{a}^{-1} is the inverse of unitary operator \hat{a} such that $\hat{a} \hat{a}^{-1} = \hat{a}^{-1} \hat{a} = 1$.

The asteric stands for the complex conjugate functions.

When the two wave function Ψ_1 and Ψ_2 are same i.e., $\Psi_1 = \Psi_2 = \Psi$ the above equation reduces to

$$\int \Psi^* (\hat{a}^{-1} \Psi) d\tau = \int (\hat{a} \Psi)^* \Psi d\tau \quad \dots(i)$$

Since \hat{a} is an eigen operator, let $\hat{a} \Psi = A \Psi$

Where A is the eigen value

Operating the operator \hat{a} on equation (i)

$$\hat{a}^{-1} \hat{a} \Psi = \hat{a}^{-1} A \hat{a} \Psi$$

$$\therefore \Psi = A \hat{a}^{-1} \Psi$$

$$\text{Or } \hat{a}^{-1} \Psi = A^{-1} \Psi$$

$$\dots(ii)$$

This implies that the eigen value of the inverse operator \hat{a}^{-1} is the reciprocal (A^{-1}) of the eigen value (A) of simple operator \hat{a} .

Multiplying both sides of the equation (ii) by Ψ^* and integrating over the whole space.

$$\int \Psi^* \hat{a}^{-1} \Psi d\tau = \int \Psi^* A^{-1} \Psi d\tau = A^{-1} \int \Psi^* \Psi d\tau \quad \dots(iii)$$

Taking the complex conjugate of each quantity in eqn. (i)

Multiplying eqn. (iv) by Ψ on both sides and integrating over all the space.

$$\int \Psi^* \hat{a}^* \Psi^* d\tau = \int \Psi^* A^* \Psi d\tau = A^* \int \Psi^* \Psi d\tau \quad \dots(v)$$

According to the condition for the unitary operator that left hand side of equation (iii) and (v) are equal

$$\text{Hence } A^{-1} \int \Psi^* \Psi d\tau = A^* \int \Psi^* \Psi d\tau \text{ or } A^{-1} = A^* A = 1$$

$$\text{Or } |A^2| = 1 \text{ or } A = 1$$

5. **Laplacian Operator.** It is represented by $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

$$\frac{\partial^2}{\partial x^2}$$

This is a common operator in quantum mechanics.

The Schrodinger equation.

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

It is used in quantum mechanics.

The Schrodinger equation viz

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} + \frac{8\pi^2 m(E-V)}{h^2} \Psi = 0$$

It in terms of Laplacian operator may be written as

$$\nabla^2 \Psi + \frac{8\pi^2 m(E-V)}{h^2} \Psi = 0$$

6 Hamiltonian operator. The Schrodinger equation $\nabla^2 \Psi + \frac{8\pi^2 m(E-V)}{h^2} \Psi = 0$

$$\Psi \frac{8\pi^2 m(E-V)}{h^2} \Psi = 0$$

$$\text{May be written as } \nabla^2 \Psi = -\frac{8\pi^2 m(E-V)}{h^2} \Psi = -\frac{8\pi^2 m}{h^2} (E\Psi - V\Psi)$$

$$\text{Or } -\frac{h^2}{8\pi^2 m} \nabla^2 \Psi + V\Psi = E\Psi$$

The above equation indicates that the operation $(\frac{h^2}{8\pi^2 m} \nabla^2 + V)$ is carried on the function Ψ .

The operator $\frac{-h^2}{8\pi^2 m} \nabla^2 + V$ is called Hamiltonian operator and is represented by \hat{H}

$$\therefore \hat{H} = \left(\frac{-h^2}{8\pi^2 m} \nabla^2 \right) + V$$

The Schrödinger wave equation may be written in another short form in terms of Hamiltonian operator.

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

Here Ψ is the eigen function and E is the eigen value.

Equal operator :- The two operators say \hat{A} and \hat{B} are called equal operator, if they operating on a function separately produces the same result

$$\text{Ex: } \frac{\partial^2}{\partial x \partial y} x^2 y = 2x \frac{\partial^2}{\partial y \partial x} x^2 y = 2x$$

Hence $\frac{\partial^2}{\partial x \partial y}$ and $\frac{\partial^2}{\partial y \partial x}$ are equal operator

Commutation of operator :- operators \hat{A} and \hat{B} commute when, $\hat{A}\hat{B}f(x) = \hat{B}\hat{A}f(x)$ [$\hat{A}\hat{B} - \hat{B}\hat{A}$] $f(x) = 0$

$[\hat{A}\hat{B} - \hat{B}\hat{A}]$ is represented by $[\hat{A}\hat{B}]$ and is called commutation of the operators \hat{A} and \hat{B} . If \hat{A} and \hat{B} commute, then $[\hat{A}, \hat{B}] = 0$ otherwise $[\hat{A}, \hat{B}] \neq 0$

$$\text{Ex: } \hat{A} = 5, \hat{B} = \frac{\partial^2}{\partial x^2} \text{ of } f(x) = x^2 + 2x$$

$$\hat{A}\hat{B}(x^2 + 2x) = 5 \cdot \frac{\partial^2}{\partial x^2}(x^2 + 2x) = 5 \cdot 2 = 10$$

$$\hat{B}\hat{A}(x^2 + 2x) = \frac{\partial^2}{\partial x^2} 5(x^2 + 2x) = \frac{\partial^2}{\partial x^2} (5x^2 + 10) = 10.$$

Hence $[\hat{A}\hat{B} - \hat{B}\hat{A}] = 0$ and \hat{A}, \hat{B} are said to be commute.

Postulates of quantum mechanics

(1) For even time independent state of system, a function of the co-ordinates can be written which is single valued, continuous and finite through out the configuration space. The function describes completely the state of the system. This function called wave function or state function, has the property that $\int_{(x_1, x_2, \dots, t)} \Psi^* \Psi d\tau$ represents the probability of finding the system in the small volume $d\tau$ of the space at time t (x_1, x_2, \dots)

$$\int_{(x_1, x_2, \dots)} \Psi^* \Psi d\tau = 1$$

Space.

(2) To each observable quantity in classical mechanics. Like position, velocity, momentum energy etc. There corresponds a certain mathematical operator in quantum mechanics.

Position	x	\hat{x}
Momentum	P_x	$\hat{P}_x = \frac{h}{2\pi i} \frac{\partial}{\partial x}$
Momentum square	\hat{P}_x	$-\frac{h^2}{4\pi^2 i^2} \frac{\partial^2}{\partial x^2}$
Kinetic energy	$T = \frac{p^2}{2m}$	$\hat{T}_x = \frac{h^2}{8\pi^2 m^2} \frac{\partial^2}{\partial x^2}$
Potential energy	$V(x)$	$\hat{V}(x)$ multiplication by $V(x)$
Total energy	$E = T_x + V(x)$	$\hat{H} = \frac{h^2}{8\pi^2 m^2} \frac{\partial^2}{\partial x^2} + V(x)$

Postulate (3) :- in any measurement of the observable properly corresponding to the operator \hat{A} , the only value that will ever be measured are the eigen value a ; which satisfy the eigen value equality,

$$\hat{A} \psi(x, t) = a \psi(x, t)$$

a , — eigen value and $\psi(x, t)$ is eigen function

Postulate (4) when a large No. of identical systems have the same wave function and with each system the observable property A is measured once, then the average value of property for all of these measurements is given as

$$\langle A \rangle = \frac{\int_{\text{all space}} \Psi^* \hat{A} \Psi dx}{\int_{\text{all space}} \Psi^* \Psi dx}$$

Postulate (5) - when state of the system becomes time dependent, i.e. Ψ and the hamiltonian are time dependent, then the wave function satisfies the time dependent schrodinger equation.

$$\hat{H}(\mathbf{x}, t) = \frac{\partial}{\partial t} \Psi(\mathbf{x}, t)$$