Operators:- An operator is a mathematical instruction or procedure to be carried out on a function so as to get another function.
It is written in the form:
(operator) . (function) = Another function.
A function on which the operation is carried out is called operand. e.g.
i) $\frac{d}{dx}(x^3) = 3x^2$. Hence $\frac{d}{dx}$ which stands for differentiation w.r.t. x is the operator, x^3 is the operand & $3x^2$ is result of operation.
ii) $\int x^3 dx = \frac{x^4}{4} + C$. Here $\int dx$, which stands for integration w.r.t. x is operator & x^3 is operand & $x^4/4 + C$ is result of operation.

Algebra of operators :- If $\hat{A}$ & $\hat{B}$ are two different operators & f is the operand then:
$(\hat{A} + \hat{B}) f = \hat{A}f + \hat{B}f$ [Addition of operators]
$(\hat{A} - \hat{B}) f = \hat{A}f - \hat{B}f$ [Subtraction of operators]

2) **Multiplication of operators :-** If $\hat{A}$ & $\hat{B}$ are two different operators & f is the operand, then expression $\hat{A}\hat{B}f$ implies that first f is operated by the operator B to get the result, say f', & then f' is operated by the operator $\hat{A}$ to get the final result say f'' i.e. $\hat{A}\hat{B}f$ implies that $\hat{B}f = f'$ & then $\hat{A}f' = f''$ so we have $\hat{A}\hat{B}f = f''$
Thus order of using operator is from right to left as written in the given expression.
If the same operation is to done a number of times in succession, It is shown by power of operator for example $\hat{A}\hat{A}f$ is written as $\hat{A}^2 f$ i.e. $\hat{A}\hat{A}f = \hat{A}^2 f$.

Commutation Relation/Rule :- It may be noted that usually
$\hat{A}\hat{B}f \neq \hat{B}\hat{A}f$
suppose $\hat{A} = x$, $\hat{B} = \frac{d}{dx}$ & $f = f(x) = x^2$ then
$\hat{A}\hat{B}f = x \cdot \frac{d}{dx}(x^2) = x(\cdot 2x) = 2x^2$
$\hat{B}\hat{A}f = \frac{d}{dx} x(x^2) = \frac{d}{dx} x^3 = 3x^2$
If, however, It is found that $\hat{A}\hat{B}f = \hat{B}\hat{A}f$
i.e. the change of order of operators give the same result, the operators are said to commute. This result is unlike the algebra where $x \times y = y \times x$ always.

The commutator of two operators $\hat{A}$ & $\hat{B}$ represented as $[\hat{A},\hat{B}]$ & is defined as: $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

If $\hat{A}\hat{B} = \hat{B}\hat{A}$, the operators are said to commute & hence $[\hat{A},\hat{B}] = 0$

NOTE:- If two operators do not commute then they cannot be determined simulteosly e.g. $[\hat{p}_x, \hat{x}] = -\frac{ih}{2\pi}$ hence momentum & position of particle cannot be determined simulteously.

3) Linear operators:- An operator $\hat{A}$ is said to be linear If for the two functions f & g

$$\hat{A}(f+g) = \hat{A}f + \hat{A}g$$

i.e. the operators on the sum of two functions gives the same result as sum of two results obtained by carrying out the same operation on the two functions separately. e.g d/dx, d^2/dx^2 etc. are linear operators whereas taking the square (SQ), taking the square root (SQRT) etc. are not linear.

Laplacian operator:- It is written by ∇^2 & is defined as:

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

Thus the Schrodinger wave eqn. viz

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{8\pi^2 m[E-V]\psi}{h^2} = 0$$

may be written as $\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi + \frac{8\pi^2 m}{h^2}[E-V]\psi = 0$

$\therefore$ In terms of Laplacian operator

$$\nabla^2\psi + \frac{8\pi^2 m}{h^2}[E-V]\psi = 0$$

Hamiltonian operator:- The Schrodinger wave eqn. written above may be be written as.

$$\nabla^2\psi = -\frac{8\pi^2 m}{h^2}[E-V]\psi$$

or $$\nabla^2\psi = -\frac{8\pi^2 m}{h^2}[E\psi - V\psi]$$

or $$-\frac{h^2}{8\pi^2 m}\nabla^2\psi = E\psi - V\psi$$

or $$\left[-\frac{h^2}{8\pi^2 m}\nabla^2 + V\right]\psi = E\psi$$

This eqn. implies that operation $\left(-\frac{h^2}{8\pi^2 m}\nabla^2+V\right)$ carried on the function ψ is equal to the total energy multiplied with the function ψ. The operator $\left(-\frac{h^2}{8\pi^2 m}\nabla^2+V\right)$ is called Hamiltonian operator & represented by $\hat{H}$.

Thus

$$\hat{H} = \frac{-h^2}{8\pi^2 m}\nabla^2 + V$$

since $\hbar = \frac{h}{2\pi}$ $\therefore$ $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V$

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

This is another short form of writing Schrodinger wave eqn. Such type of function i.e. ψ is called eigen function & E is called eigen value. Such an eqn. is therefore called eigen value eqn.

[Contd.... on Pg (5)]

Num:- Prove that $[\hat{A},\hat{B}] = -[\hat{B},\hat{A}]$

Sol:- Since $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = -\hat{B}\hat{A} + \hat{A}\hat{B}$

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

Num:- evaluate the commutator $\left[x^2, \frac{d^2}{dx^2}\right]$

Sol:- suppose the operand is $\psi(x)$, then

$$\left[x^2, \frac{d^2}{dx^2}\right]\psi(x) = \left[x^2\frac{d^2}{dx^2} - \frac{d^2}{dx^2}x^2\right]\psi(x)$$

$$= \left\{x^2\frac{d^2\psi}{dx^2} - \frac{d^2}{dx^2}(x^2\psi)\right\} = x^2\frac{d^2\psi}{dx^2} - \frac{d}{dx}\frac{d}{dx}(x^2\psi)$$

$$= x^2\frac{d^2\psi}{dx^2} - \frac{d}{dx}\left[x^2\frac{d\psi}{dx} + \psi(2x)\right]$$

$$= \cancel{x^2\frac{d^2\psi}{dx^2}} - \left[\cancel{x^2\frac{d^2\psi}{dx^2}} + (2x)\frac{d\psi}{dx} + \frac{d\psi}{dx}(2x) + 2(\psi)\right]$$

$$= -2\psi - 4x\frac{d\psi}{dx} = \left(2 - 4x\frac{d}{dx}\right)\psi$$

$$\therefore \left[x^2, \frac{d^2}{dx^2}\right] = -2 - 4x\frac{d}{dx}$$

Num:- Prove that $[\hat{A}^2,\hat{B}] = \hat{A}[\hat{A},\hat{B}] + [\hat{A},\hat{B}]\hat{A}$

Sol:- R.H.S $= \hat{A}[\hat{A}\hat{B} - \hat{B}\hat{A}] + [\hat{A}\hat{B} - \hat{B}\hat{A}]\hat{A}$

$$= \hat{A}^2\hat{B} - \cancel{\hat{A}\hat{B}\hat{A}} + \cancel{\hat{A}\hat{B}\hat{A}} - \hat{B}\hat{A}^2$$

$$= \hat{A}^2\hat{B} - \hat{B}\hat{A}^2 = [\hat{A}^2,\hat{B}]$$

Num:- Prove that $\left[x, \frac{d}{dx}\right] = -1$ (4)

Sol:- Suppose $\psi(x)$ is an operand then

$$\left[x, \frac{d}{dx}\right]\psi(x) = \left[x\frac{d}{dx} - \frac{d}{dx}x\right]\psi(x)$$

$$= x\frac{d\psi}{dx} - \frac{d}{dx}(x\psi) = \cancel{x\frac{d\psi}{dx}} - \cancel{x\frac{d\psi}{dx}} - \psi \cdot 1$$

$$= -\psi$$

Removing ψ from both sides

$$\left[x, \frac{d}{dx}\right] = -1$$

Num:- Find the expression for the operator $\left(\frac{d}{dx}x\right)^2$

Sol:- Suppose $\psi(x)$ is an operand then

$$\left(\frac{d}{dx}x\right)^2\psi(x) = \left(\frac{d}{dx}x\right)\left(\frac{d}{dx}x\right)\psi = \left(\frac{d}{dx}x\right)\left(\frac{d}{dx}x\psi\right)$$

$$= \left(\frac{d}{dx}x\right)\left(x\frac{d\psi}{dx} + \psi\right) = \frac{d}{dx}\left(x^2\frac{d\psi}{dx} + x\psi\right)$$

$$= 2x\frac{d\psi}{dx} + x^2\frac{d^2\psi}{dx^2} + \psi + x\frac{d\psi}{dx}$$

$$= x^2\frac{d^2\psi}{dx^2} + 3x\frac{d\psi}{dx} + \psi$$

$$= \left(x^2\frac{d^2}{dx^2} + 3x\frac{d}{dx} + 1\right)\psi$$

Removing ψ from both sides

$$\left(\frac{d}{dx}x\right)^2 = x^2\frac{d^2}{dx^2} + 3x\frac{d}{dx} + 1$$

Num:- Show that the commutator $[\hat{x}^n, \hat{p}_x] = i\hbar n x^{n-1}$ where n is a positive integer.

Sol.- $$[\hat{x}^n, \hat{p}_x]f = [x^n p_x - p_x x^n]f = \left[x^n\left(-i\hbar\frac{\partial}{\partial x}\right) - \left(-i\hbar\frac{\partial}{\partial x}\right)x^n\right]f$$

$$= -x^n i\hbar\frac{\partial f}{\partial x} + i\hbar\frac{\partial}{\partial x}(x^n f)$$

$$= i\hbar\left[-\cancel{x^n\frac{\partial f}{\partial x}} + n x^{n-1} f + \cancel{x^n\frac{\partial f}{\partial x}}\right] = i\hbar n x^{n-1} f$$

Removing f from both sides of the eqn. we get

$$[\hat{x}^n, \hat{p}_x] = i\hbar n x^{n-1}$$