An operator is a symbol that designates a process that will transform one function into another function.

For example: An operator Dx given as follows

Dx = d /dx

Means a first derivative of function f(x) with respect to x should be taken.

If two or more operators are applied simultaneously to a function, the operator immediately adjacent to the function will operate on the function first, giving a new function.

For example: If Dx = d /dx and Dy = d/dx to the function f(x,y) = x^3y^2.

Dx Dy (x^3y^2) = Dx (2 x^3y) = 6 x^2 y

Or

Dy Dx (x^3y^2) = Dy (3 x^2y^2) = 6 x^2 y

The result of the two operations is independent of the order in which the operators are applied, then these operators are said to commute.

That is

Dx Dy f(x,y) = Dy Dx f(x,y)

Or

[Dx Dy - Dx Dy] f(x,y) = o

Here the [ ] brackets are called as commuter brackets, and the expression in the bracket itself an operator called the commutator of the operators.

In general we can say that two operators A and B commute if and only if

[AB - BA] f(x) =0

Quantum-Mechanical Operators:

The Schrödinger equation of a particle of mass m confined to a thre-dimensional region and with a potential energy U(x,y,z) is given as follow:

$$\frac{-h^2}{8\pi^2 m}\left(\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2}\right) + [U(x,y,z)]\,\psi = \varepsilon\psi$$

The mathematical expression for ψ that satisfies this equation generally exist only for certain values of ε and these values are the energies of the states of the system.

We can write the above equation as:

$$\left\{\frac{-h^2}{8\pi^2 m}\left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2}\right) + [U(x,y,z)]\right\}\psi = \varepsilon\psi$$

The expression in the curly bracket is an example of an quantum mechanical operator and is known as Hamiltonian operator and its symbol is H. The “ ^ “ ; “hat” signifies it as a operator.

Thus the equation can be written as:

$$H\psi = \varepsilon\psi$$

The function which satisfies such equations are called as “eigenfunctions” and the values of constants calculated from such equations are called as “eigenvalues”.

Eigen is a German word, and it means characteristic.

Postulates of Quantum Mechanics:

The wave functions from the Schrödinger equation or eigen functions from the operator equation can be used to deduce the information about the systems in each of allowed states.

Thus, we introduce a set of 'postulates' that are expressed in terms of quantum-mechanical operators.

1. The value of each physical property can be deduced by operating on eigenfunctions with the operator corresponding to that physical property. or by solving Schrödinger equation.

2. There are two basic operator which can be used to deduce physical properties.

   a. Position Operator is for one dimensional system and it is the position coordinate of the system.

   Position Operator = x = x

   b. The momemtum operator in x direction is

   Momentum operator = p = (h / 2 π i) d /dx

3. There are two different situations arises when we a value of any physical property is obtained by working on eigen functions:

a. When quantized values are obtained:

For a particular physical property, the operator A is such that

$$A\psi = a\psi$$

Where a is the number of allowed values of physical property.

For example, when the Hamiltonian operator is used, $H\psi = \varepsilon\psi$ yields the values for ε. Any measurement of the system would show that it had an energy equal to one of the ε values.

b. When average values are obtained:

For a another physical property, the operator B is such that

$$B\psi \neq b\psi$$

Where <b> is average value of physical property obtained as

$$\langle b \rangle = \int \psi B \, dT \, / \int \psi^2 \, dT$$

For, e.g. in the particle-on-line problem, the particle is not restricted to certain positions along the line, but we can find out the average position of the particle using above expression.

A derived operator for kinetic energy:

Operators for the other physical properties can be deduced from the position and momentum operators.

Kinetic energy is given as :

$$KE = m\upsilon^2 / 2 = (m\upsilon)^2 / 2m = (\text{momentum})^2 / 2m$$

Thus the kinetic energy operator, T is given as

Kinetic-energy operator = T

$$= 1 / 2m \, [(h / 2 \pi i) \, d /dx] \, [(h / 2 \pi i) \, d /dx]$$

$$= (- h^2 / 8 \pi^2 m) \, d^2 /dx^2$$

For three-dimensional system

Kinetic-energy operator = T

$$= (- h^2 / 8 \pi^2 m) [d^2 /dx^2 + d^2 /dy^2 + d^2 /dz^2]$$

Rotation in a plane:
Angular Features:

Angular momentum is an important physical property of atoms and molecules.

Angular momentum values are used to characteristics the electronics states of atoms and some molecules and for the rotational states of the molecules of gas.

Angular Momentum Operators:

Similar to kinetic energy operators angular momentum operators can be deduced from the basic position operator and linear momentum operator.

The direction and the magnitude of the angular momentum can be described by a vector.

This vector is perpendicular to the plane that contains he radius vector and the linear momentum vector.

Refer figure 9-7

Refer 9-6

The magnitude of this vector, since the radius and linear momentum vector are perpendicular to each other, is equal to the product of the magnitudes of these two vectors.

This can be expressed in term of coordinates x and y of particle and the values of angular momentum components P_x and P_y.

Thus the contribution to the angular momentum along the z directions are xP_y and $-yP_x$.

Thus,
The angular momentum , $L_z = x P_y - y P_x$

Thus, in order to get the value of angular momentum operator, L_z,

We use position operator x = x and y = y and
linear momentum operators $P_x = (h / 2 \pi i) /(d /dx)$ and
$P_y = (h / 2 \pi i) /(d /dy)$

Thus, we get

Angular momentum operator $= L_z$

$$= (h / 2 \pi i) [x (d/ dy) - y (d/dx)]$$

The polar coordinates are more convenient than Cartesian coordinates to calculate the angular momentums.

Refer figure 9-8

Thus,

$x = r \cos ø$

and

$dx / dø = -r \sin ø = -y$

Also,

$y = r \sin ø$

and

$dy / dø = r \cos ø = x$

In addition, the derivative df / dø of any function f with respect to ø can be written in terms of x and y as follows.

$$df / dø = (df / dx) (dx / dø) + (df / dy) (dy / dø)$$

but

$$dx / dø = -y \quad \text{and} \quad dy / dø = x$$

Therefore

$$df / dø = (df / dx) (-y) + (df / dy) (x)$$

$$df / dø = x (df / dy) - y (df / dx)$$

Thus, in general we can write

$$d / dø = x (d / dy) - y (d / dx)$$

Therefore the angular momentum operator L_z can be written in terms of its polar coordinates:

Angular momentum operator $= L_z = (h / 2 \pi i) (d / dø)$

Rotational Kinetic Energy Operator:

The kinetic energy can be expressed in terms of angular velocity ω.

$$\omega = 2\pi\nu$$

$$= 2\pi \times \upsilon / (2\pi r)$$

$$= \upsilon / r$$

The moment of Inertia = $I = mr^2$

Therefore, we can write

$$KE = (1/2)\, m\upsilon^2$$

$$= (1/2)\,(m r^2)\,(\upsilon / r)^2$$

$$= (1/2)\,(I)\,(\omega)^2$$

$$= (I\,\omega)^2 / 2I$$

Thus, the we can express KE operator T_z as

$$Tz = (h^2 / 8\pi^2 I)\,(d^2 / d^2ø)$$