Study Notes on Quantum Operators and Functions

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QUANTUM OPERATORS & FUNCTIONS

OPERATORS

An operator is a symbol which is used to express mathematical calculations / procedures / commands in which one function changes to another one.

Operator (Function) = New Function

Algebra of Operators

1. **Addition and Subtraction of Operators:** If $\hat{A}$ and $\hat{B}$ are two different operators and *f(x)* is the function, then,

$$\left(\hat{A}+\hat{B}\right) f(x)=\hat{A}f(x)+\hat{B}f(x)$$

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

2. **Multiplication of Operators:** If $\hat{A}$ and $\hat{B}$ are two different operators and *f(x)* is the function, then order of the operation is very important and it can be represented as:

$$\hat{A}\hat{B}[f(x)]=\hat{A}\left[\hat{B}f(x)\right]=\hat{A}[f'(x)]=f''(x) \qquad \text{(Here, } \hat{B}f(x)=f'(x))$$

The first operator $\hat{B}$ operates on function *f(x)* which produces *f′(x)* and then operator $\hat{A}$ operates on function *f′(x)* which produces *f″(x)*.

3. **Commutative Property:** If two operators are such that the result of their successive applications remains same irrespective of the order of operations, then the two operators are said to be commutative.

If, $\hat{A}\hat{B}f[(x)]=\hat{B}\hat{A}f'[(x)],$, then the two operators $\hat{A}$ and $\hat{B}$ commute with each other i.e., the normal product of two operators is equal to their product in reverse order.

The expression $[\hat{A}\hat{B}-\hat{B}\hat{A}]$ is called **commutator** and is represented as $[\hat{A}\bullet\hat{B}]$.

Commutator= $[\hat{A}\bullet\hat{B}]=\hat{A}\hat{B}[f(x)]-\hat{B}\hat{A}[f(x)]$

If the two operators commute with one another, then the value of commutator is zero, i.e.,

$$[\hat{A}\bullet\hat{B}]=\hat{A}\hat{B}[f(x)]-\hat{B}\hat{A}[f(x)]=0$$

Significance of Commutation: If the two operators commute, then expression will be as follows:

$$[\hat{A} \bullet \hat{B}] = \hat{A}\hat{B}[f(x)] - \hat{B}\hat{A}[f(x)] = 0$$

If the two operators do not commute, then,

$$[\hat{A} \bullet \hat{B}] = \hat{A}\hat{B}[f(x)] - \hat{B}\hat{A}[f(x)] \neq 0$$

Eigen Function, Eigen Value and Eigen value Equation: If an operator $\hat{A}$ operates on a well-behaved function *f(x)*, and gives the same function multiplied by a constant. Then, the function *f(x)* is called the eigen function and the constant is called the eigen value of the operator. The equation formed is called as Eigen Value Equation i.e.,

$$\boxed{\hat{A}\underset{\substack{\downarrow \\ \text{eigen function}}}{f(x)} = \underset{\substack{\downarrow \\ \text{eigen value}}}{a} f(x)}$$

$$\frac{d}{dx}\underset{\substack{\downarrow \\ \text{eigen function}}}{(e^{ax})} = \underset{\substack{\downarrow \\ \text{eigen value}}}{a} e^{ax}$$

Some of the Common Operators used in Quantum Mechanics:

1. Laplacian Operator (∇^2) : It is an important differential operator used in quantum mechanics and it can be represented as:

$$\nabla = \hat{i}\frac{\partial}{\partial x} + \hat{j}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}$$

Here, $\hat{i}, \hat{j}$ and $\hat{k}$ are unit vectors along x, y and z axes respectively.

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \qquad (\hat{i}\cdot\hat{i} = \hat{j}\cdot\hat{j} = \hat{k}\cdot\hat{k} = 1)$$

2. Momentum Operator $(\hat{p})$:

$$\hat{p}_x = \frac{h}{2\pi i}\frac{\partial}{\partial x} = \frac{\hbar}{i}\frac{\partial}{\partial x} = -i\hbar\frac{\partial}{\partial x} \qquad \left(\text{Here, } \hbar = \frac{h}{2\pi}\right)$$

Similarly,

$$\hat{p}_y = \frac{h}{2\pi i}\frac{\partial}{\partial y} = \frac{\hbar}{i}\frac{\partial}{\partial y} = -i\hbar\frac{\partial}{\partial y}$$

$$\hat{p}_z = \frac{h}{2\pi i}\frac{\partial}{\partial z} = \frac{\hbar}{i}\frac{\partial}{\partial z} = -i\hbar\frac{\partial}{\partial z}$$

3. Square of Momentum Operator $(\hat{p}^2)$:

$$\hat{p}_x^2 = \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) = -\hbar^2\frac{\partial^2}{\partial x^2} \qquad (i \times i = i^2 = -1)$$

$$\hat{p}_y^2 = \left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right)\left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right) = -\hbar^2\frac{\partial^2}{\partial y^2}$$

$$\hat{p}_z^2 = \left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right)\left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right) = -\hbar^2\frac{\partial^2}{\partial z^2}$$

4. Angular Momentum Operator $(\hat{L})$: Angular momentum is given by the vector product of position $(\vec{r})$ and their linear momentum $(\vec{p})$.

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

$$\vec{p} = p_x\hat{i} + p_y\hat{j} + p_z\hat{k}$$

Here, $\hat{i}$, $\hat{j}$ and $\hat{k}$ are unit vectors along *x, y* and *z* axes respectively.

Now, $\vec{L} = \vec{r} \times \vec{p}$

$$\vec{L} = (x\hat{i} + y\hat{j} + z\hat{k}) \times (p_x\hat{i} + p_y\hat{j} + p_z\hat{k})$$

$$= \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

$$\vec{L} = \hat{i}(yp_z - zp_y) - \hat{j}(xp_z - zp_x) + \hat{k}(xp_y - yp_x)$$

$$\vec{L} = \hat{i}(yp_z - zp_y) + \hat{j}(zp_x - xp_z) + \hat{k}(xp_y - yp_x) \quad \text{..... (3.13)}$$

Also, by definition

By definition $\vec{L} = L_x\hat{i} + L_y\hat{j} + L_z\hat{k}$

5. Kinetic Energy Operator $(\hat{T})$:

$$\hat{T} = -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right]$$

$$\hat{T} = -\frac{\hbar^2}{2m}\nabla^2$$

6. Hamiltonian Operator $(\hat{H})$: The total energy of a system is the sum of kinetic and potential energies. The operator which corresponds to the total energy is called Hamiltonian operator $(\hat{H})$.

Total energy of a system containing a particle of mass ‘m’ is given as:

E = K.E. + P.E.

$$\hat{H} = \hat{T} + \hat{V}$$

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(x, y, z)$$

In quantum mechanics we deal with only **Linear Hermitian Operators:**

1. Linear Operators: If it is applied on the sum of two functions, then the result is equal to the sum of the operations on the two functions separately.

   Let operator $\hat{A}$ operates on two functions of f and g, then,

$$\hat{A}[f + g] = \hat{A}f + \hat{A}g$$

2. Hermitian Operators: Suppose ψ and ϕ are the two eigen functions of the operators $\hat{A}$ and if

$$\int_{-\infty}^{+\infty} \Psi^*(\hat{A}\phi)d\tau = \int_{-\infty}^{+\infty} \phi(\hat{A}\psi)^* d\tau$$

   then the operator $\hat{A}$ is called Hermitian operator.

   Two properties of Hermitian Operator are:

   (i) Eigen Values of Hermitian Operators are Real (Positive or Negative).
   (ii) Eigen Functions of a Hermitian Operator Corresponding to different Eigen values are Orthogonal.

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