S. S. College. Jehanabad (Magadh University)

Department : Physics

Subject : Quantum Mechanics

Class : B.Sc(H) Physics Part III

Topic: Formal Structure of Quantum Mechanics

Teacher : M. K. Singh

The Formal Structure of Quantum Mechanics

- The Dirac Notation

It is very convenient and compact Notation for the Scalar product of two functions. The scalar product of two functions $\psi_1(\vec{r})$ and $\psi_2(\vec{r})$ is denoted by the symbol $\langle\psi_1|\psi_2\rangle$:

$$\langle\psi_1|\psi_2\rangle = \int \psi_1^*(\vec{r})\,\psi_2(\vec{r})\,d\vec{r}$$

↳ Dirac Notation

- The object $|\psi_2\rangle$ is known as a ket vector.
- The object $\langle\psi_1|$ is known as a bra vector.
- They join together to form the "bra-ket" as $\langle\psi_1|\psi_2\rangle$.

$$\langle\psi_2|\psi_1\rangle = \langle\psi_1|\psi_2\rangle^*$$
$$\langle\psi_1|c\psi_2\rangle = c\langle\psi_1|\psi_2\rangle$$
$$\langle c\psi_1|\psi_2\rangle = c^*\langle\psi_1|\psi_2\rangle$$
$$\langle\psi_3|\psi_1+\psi_2\rangle = \langle\psi_3|\psi_1\rangle + \langle\psi_3|\psi_2\rangle$$

where c is a complex number and ψ_3 is a third function.

$$|\psi_1\rangle^* = \langle\psi_1|$$

$$|\psi_2\rangle^* = \langle\psi_2|$$

Operators :-

An operator transforms one function into another. If an operator $\hat{A}$ transforms the function ψ into the function ϕ, then we write:

$$\hat{A}\psi = \phi$$

example :-

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

It indicates that the operator $\hat{A}$ multiply the function $\psi(x)$ by x.

Similarly,

$$\hat{A}\psi(x) = \frac{d}{dx}\psi(x)$$

$$\hat{A} \equiv \frac{d}{dx}$$

- An operator is said to be linear if it satisfies

$$\hat{A}[\psi_1+\psi_2] = \hat{A}\psi_1 + \hat{A}\psi_2 \quad —(1)$$

and

$$\hat{A}[c\psi] = c\hat{A}\psi \quad —(2)$$

These two eq (1) & (2), will give

$$\hat{A}[c_1\psi_1 + c_2\psi_2] = c_1\hat{A}\psi_1 + c_2\hat{A}\psi_2$$

condition for linearity

Ortogonal states :-

Two kets $|\psi_1\rangle$ and $|\psi_2\rangle$ are said to be orthogonal if they vanishing scalar Product

$$\langle\psi_1|\psi_2\rangle = 0$$

Orthonoomal states :-

Two kets $|\psi_1\rangle$ and $|\ \rangle$ are said to be orthonormal if they are orthogonal and if each one of them has a unit foom:

$$\langle\psi_1|\psi_2\rangle = 0 \ \& \ \langle\psi_1|\psi_1\rangle = 1$$
$$\langle\psi_2|\psi_2\rangle = 1$$

• Forbidden quantities :-

1) If $|\psi_1\rangle$ and $|\psi_2\rangle$ belongs to same vector space, Then the Product of

(i) $|\psi_1\rangle|\psi_2\rangle \rightarrow$ Forbidden

(ii) $\langle\psi_1|\langle\psi_2| \rightarrow$ Forbidden

• Hermitian Adjoint :-

The Hermitian Adjoint or conjugate is given by If $\hat{A}^{+} = \hat{A}$

$$\langle\psi_1|\hat{A}|\psi_2\rangle = \langle\psi_1|\hat{A}^{+}|\psi_2\rangle$$

Properties of Hermitian conjugate/Adjoint

1) $(\hat{A}^{+})^{+} = \hat{A}$ 2) $(a\hat{A})^{+} = a^{*}\hat{A}^{+}$

3) $(\hat{A}^{n})^{+} = (\hat{A}^{+})^{n}$ 4) $(\hat{A}\hat{B}\hat{C}\hat{D})^{+} = \hat{D}^{+}\hat{C}^{+}\hat{B}^{+}\hat{A}^{+}$

Hermitian & Skew-Hermitian operators

Hermitian :

$$\hat{A} = \hat{A}^{+} \text{ or } \langle\psi_1|\hat{A}|\psi_2\rangle = \langle\psi_2|\hat{A}|\psi_1\rangle^{*}$$

Skew-Hermitian operators :

$$\hat{B}^{+} = -\hat{B} \text{ or } \langle\psi_1|\hat{B}|\psi_2\rangle = -\langle\psi_2|\hat{B}|\psi_1\rangle^{*}$$

Q. Prove that $\hat{P} = -i\hbar\vec{\nabla}$ is hermitian.

Solution:

$$\langle\psi|\hat{P}|\psi\rangle = \int\langle\psi|\hat{P}|\psi\rangle\, d\gamma$$

$$= \int\vec{\psi}^*(-i\hbar\vec{\nabla}\psi)\, d\vec{\gamma}$$

$$\int\psi^*(-i\hbar\vec{\nabla}\psi)d\vec{r} = -i\hbar\int(\vec{\psi}^*\vec{\nabla}\psi)\, d\vec{\gamma} \quad — (1)$$

$$\Rightarrow \int\psi^*\vec{\nabla}\psi\, d\vec{r} = +i\hbar\int(\vec{\nabla}\psi^*)\,\psi\, d\vec{\gamma} \quad — (2)$$

$$\int\psi^*\vec{\nabla}\psi\, d\gamma = -\int(\vec{\nabla}\psi^*)\,\psi\, d\vec{\gamma} \quad — (3)$$

Integrating left hand integral by parts

$$\int\psi^*\vec{\nabla}\psi\, d\gamma = \psi^*\psi\Big|_{-\infty}^{\infty} - \int(\vec{\nabla}\psi^*)\,\psi\, d\gamma \quad — (4)$$

from (3) & (4), we get $\hat{P}$ is hermitian observator