Quantum Mechanics

Lecture #4

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Hermition Operator:

"Hermition Operators"

"In quantum mechanics, there are special type of operators called "Hermition operators"."

$\because A = A^*$

- They have the property that all of their eigen values are real (not complex).
- All observable properties are represented by Hermition operators (but not all Hermition operators correspond to an observable property).

Eigen values of Hermition operator are real & prove.

Hermiticity is defined as

$$\hat{A}\psi_\alpha = a_\alpha \psi_\alpha$$

where

- ψ_α is the α^{th} eigen function of A.

Cont.

- a_α is the eigen value of ψ_α
left multiply by ψ_α^* and integrate

$$\int \psi_\alpha^* \hat{A} \psi_\alpha \, d\tau = a_\alpha \int \psi_\alpha^* \psi_\alpha \, d\tau$$

$\Rightarrow \int \psi_\alpha^* \psi_\alpha \, d\tau = 1$ because of normalization.

$\Rightarrow \int \psi_\alpha^* \hat{A} \psi_\alpha \, d\tau = \left\{ \int \psi_\alpha^* \hat{A} \psi_\alpha \, d\tau \right\}^*$ because of hermiticity

$\therefore \int \psi_\alpha^* \hat{A} \psi_\alpha \, d\tau = a_\alpha = a_\alpha^* = \left\{ \int \psi_\alpha^* \hat{A} \psi_\alpha \, d\tau \right\}^*$

Hence

$a_\alpha = a_\alpha^*$ which is true only if a_α is real.

Prove that P_x is hermition operator Momentum

$$\int_a^b (\hat{P}_x \psi_1)^* \psi_2 \, d\tau = \int_a^b \psi_1^* \hat{P}_x \psi_2 \, d\tau$$

taking

$$\text{L.H.S} = \int_a^b (\hat{P}_x \psi_1)^* \psi_2 \, d\tau$$

$$= \int_a^b \left(-i\hbar \frac{\partial}{\partial x} \psi_1 \right)^* \psi_2 \, d\tau$$

$$= i\hbar \int_a^b \frac{\partial}{\partial x} \psi_1^* \psi_2 \, d\tau$$

Cont.

$$= i\hbar \left[\psi_1^* \psi_2 \Big|_a^b - \int_a^b \psi_1^* \frac{\partial \psi_2}{\partial x} d\tau \right]$$

we assume that

$$\psi_1^* \psi_2 \Big|_a^b = 0$$

So,

$$L.H.S = 0 - i\hbar \int_a^b \psi_1^* \frac{\partial \psi_2}{\partial x} d\tau$$

$$= \int_a^b \psi_1^* \left(-i\hbar \frac{\partial}{\partial x}\right) \psi_2 \, d\tau$$

$$= \int_a^b \psi_1^* \hat{P}_x \psi_2 \, d\tau$$

$= R.H.S.$

Hence proved.

Conditions of Hermition operator:

Conditions of Hermition Operator :-

If an operator is hermition operator it should satisfy

i) $\left(\int \psi^* A \psi \, d\tau\right)^* = \int \psi^* A \psi \, d\tau$

ii) $\int (A\psi^*) \psi \, d\tau = \int \psi^* A \psi \, d\tau$ ⇒ most imp. (transpose)

iii) $(A\psi, \psi) = (\psi, A\psi)$

or

$(A\psi, \phi) = (\phi, A\psi)$

Theorem:

Note :- $\langle A \rangle = \int \psi^* \hat{A} \psi \, d\tau = (\psi, A\psi) = \langle \psi | A | \psi \rangle$

Theorem :- Show that eigen functions belonging to the diff. eigen values of a given hermition operator are orthogonal.

let

$$\overset{\text{operator}}{\alpha} U_m = \overset{\text{eigen value}}{a_m} \overset{\text{eigen fn.}}{U_m} \quad \text{---} \quad (i)$$

$$\alpha U_n = a_n U_n \quad \text{---} \quad (ii)$$

From transpose property of H.O

$$\int (\alpha U_m)^* U_n \, d\tau = \int U_m^* \alpha U_n \, d\tau$$

$$\Rightarrow \int (a_m U_m)^* U_n \, d\tau = \int U_m^* \alpha U_n \, d\tau$$

$$\Rightarrow \int U_m^* a_m^* U_n \, d\tau = \int U_m^* a_n U_n \, d\tau$$

or

$$a_m^* \int U_m^* U_n \, d\tau = a_n \int U_m^* U_n \, d\tau$$

$\because a_m^* = a_m$ For eigen value

$$a_m \int U_m^* U_n \, d\tau = a_n \int U_m^* U_n \, d\tau$$

$$(a_m - a_n) \int U_m^* U_n \, d\tau = 0$$

so, either $a_m - a_n = 0 \rightarrow a_m = a_n$ which is no possible.

or $\int U_m^* U_n \, d\tau = 0$

$$\boxed{\int U_m^* U_n \, d\tau = 0}$$

Adjoint of Operator:

- **Adjoint of an operator :-**

Suppose 'A' is an arbitrary operator, not necessarily H.O then adjoint (read as Dagger) is

- $\int \psi^* A^\dagger \phi \, d^3r = \int (A\psi)^* \phi \, d^3r$ $\quad \because dV = d^3r = dx\,dy\,dz$
- $(\psi, A^\dagger \phi) = (A\psi, \phi)$ $\quad \Rightarrow A^\dagger = (A)^*$ (conjugate + transpose)

Unitary Operators:

- **Unitary Operators** :- "A linear operator whose inverse (Adjoint) is its adjoint is called unitary."

$$U^{-1} = U^{t}$$

It helps us to generalize the complex numbers whose absolute value is 1.

$$UU^{t} = U^{t}U = I$$

This will lead us to a identity value.

Properties :-
- It should be adjoint operator.
- Like Hermition operators, the eigen vectors of a unitary matrix are orthogonal.
- Its eigenvalues are not necessarily real.

If we take conjugate and then transpose the answer must be unity. Thats why it is called unitary operators.

Simultaneous measurement and commutators:

Simultaneous measurement and Commutators :-

If A, B are two linear operators corres- ponding to any dynamical observeable

$$A\psi = a\psi \quad , \quad B\psi = b\psi$$

"ψ" is called "Simultaneous eigen function."

Now

$$BA\psi = B(a\psi) = Ba\psi = aB\psi \quad \text{--- (i)}$$
$$AB\psi = A(b\psi) = Ab\psi = bA\psi \quad \text{--- (ii)}$$

(ii) − (i)

$$(AB - BA)\psi = bA\psi - aB\psi$$
$$(AB - BA)\psi = 0$$

This is condition of simultaneous.
This condition is not satisfied only if operators are not commute.

Note :-

If the wave fn. is same and on same level we want to fix two different quantities than these are simultaneous measurements.

Commutators in Quantum Mechanics:

Since the definite value of observable A can be assigned to a system only if the system is in an eigenstate of $\hat{A}$, same in the case of two observables A and B. Suppose the system has a value of A_i for observable A and B_j for observable B. Then

$$\hat{A}\psi_{A_i,B_j} = A_i \psi_{A_i,B_j} \quad \text{--- (i)}$$

$$\hat{B}\psi_{A_i,B_j} = B_j \psi_{A_i,B_j} \quad \text{--- (ii)}$$

Multiply eq. (i) by '$\hat{B}$' and (ii) by '$\hat{A}$'

$$\Rightarrow \hat{B}\hat{A}\psi_{A_i,B_j} = \hat{B}A_i\psi_{A_i,B_j} \quad \text{--- (iii)}$$

$$\Rightarrow \hat{A}\hat{B}\psi_{A_i,B_j} = \hat{A}B_j\psi_{A_i,B_j} \quad \text{--- (iv)}$$

Using fact that ψ_{A_i,B_j} is an eigen state of $\hat{A}$ and $\hat{B}$ then

$$\hat{B}\hat{A}\psi_{A_i,B_j} = A_i B_j \psi_{A_i,B_j} \quad \text{(By eq. i)}$$

$$\hat{A}\hat{B}\psi_{A_i,B_j} = B_j A_i \psi_{A_i,B_j} \quad \text{(By eq. ii)}$$

By subtracting

$$(\hat{A}\hat{B} - \hat{B}\hat{A})\psi_{A_i,B_j} = 0$$

Cont.

or $\hat{A}\hat{B} = \hat{B}\hat{A}$

or $[\hat{A}, \hat{B}] = 0$

⇒ For two physical quantities to be simultaneously observable, their operator representation must commute.

⇒ Rules :- Some rules are used for the evaluation of commutators:

(i) $[\hat{A}, \hat{B}] + [\hat{B}, \hat{A}] = 0$

(ii) $[\hat{A}, \hat{A}] = 0$

(iii) $[\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]$

(iv) $[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$

(v) $[\hat{A}\hat{B}, \hat{C}] = [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}]$

(vi) $[\hat{A}, [\hat{B}, \hat{C}]] + [\hat{C}, [\hat{A}, \hat{B}]] + [\hat{B}, [\hat{C}, \hat{A}]] = 0$

(vii) If $\hat{A}$ and $\hat{B}$ operators which commute with their commutators

$$[\hat{A}, \hat{B}^n] = n\hat{B}^{n-1}[\hat{A}, \hat{B}]$$

$$[\hat{A}^n, \hat{B}] = n\hat{A}^{n-1}[\hat{A}, \hat{B}]$$

Cont.

(viii) If $[\hat{A}, \hat{B}] = i\hat{C}$ the uncertainties in A and B defined as

$$\Delta A^2 = \langle A^2 \rangle - \langle A \rangle^2$$

Obey relation

$$(\Delta A)(\Delta B) \geq \frac{1}{2} |\langle C \rangle|$$

=> which is Heisenberg uncertainty principle.
It is easy to derive

$$(\Delta x)(\Delta P_x) \geq \frac{\hbar}{2}$$

From this generalized rule.

- we have the identity (used for coupled-cluster theory):

$$e^{\hat{A}} \hat{B} e^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}] + \frac{1}{2!}[\hat{A}, [\hat{A}, \hat{B}]] + \frac{1}{3!}[\hat{A}, [\hat{A}, [\hat{A}, \hat{B}]]] + \dots$$

Proof that the eigenvalues of Hermition operators are real.

(In Dirac notation)

$A|\psi\rangle = a|\psi\rangle$

$\langle\psi|A|\psi\rangle = \langle\psi|a|\psi\rangle = a\langle\psi|\psi\rangle = a \quad \because \langle\psi|\psi\rangle = 1$

$(\langle\psi|A|\psi\rangle)^* = a^*(\langle\psi|\psi\rangle)^* = a^*$

$\langle\psi|A|\psi\rangle = (\langle\psi|A|\psi\rangle)^*$ by Hermiticity

$\therefore a = a^*$ only true if a is real.