Lecture-11

Schmidt Orthogonalization Procedure:-

Statement:-

Let T be a Hermitian operator. ψ_k be a wave fn. which is linear combination of ψ_i & ψ_j. Let λ be some eigenvalue of ψ_i & ψ_j. Then prove that

$$\psi_k = \frac{\psi_j - \psi_i(\psi_i, \psi_j)}{\sqrt{1 - |(\psi_i, \psi_j)|^2}}$$

, under two conditions, when ψ_i is orthogonal to ψ_k & ψ_i ~~&~~ ψ_j & ψ_k are normalized wave fns.

Proof:-

As ψ_k is linear combination of ψ_i & ψ_j i.e $\psi_k = c_1\psi_i + c_2\psi_j$, where c_1 & c_2 are real constants.

As T is an operator, ψ_i & ψ_j with some eigenvalue λ, Then

$T\psi_i = \lambda\psi_i$, $T\psi_j = \lambda\psi_j$, Then

$T\psi_k = T(c_1\psi_i + c_2\psi_j) = c_1 T\psi_i + c_2 T\psi_j$

$= c_1\lambda\psi_i + c_2\lambda\psi_j$

so $T\psi_k = \lambda(c_1\psi_i + c_2\psi_j)$

$\Rightarrow \lambda$ is eigenvalue of ψ_k.

This function is on two fold degeneracy. We can extend it

we are given two conditions, as

$(\psi_i, \psi_k) = 0$ —(1)

(1) ⇒ $\int \psi_i^* (c_1\psi_i + c_2\psi_j)\, dx = 0$

$c_1 \int |\psi_i|^2 dx + c_2 (\psi_i, \psi_j) = 0$

$c_1 = -c_2 (\psi_i, \psi_j)$

$(\psi_k, \psi_k) = 1$ —(2)

(2) ⇒ $\int (c_1\psi_i + c_2\psi_j)^* (c_1\psi_i + c_2\psi_j)\, dx = 1$

$\int (c_1\psi_i^* + c_2\psi_j^*)(c_1\psi_i + c_2\psi_j)\, dx = 1$

$(c_1)^2 (1) + (c_2)^2 (1) + c_1 c_2 (\psi_i, \psi_j) + c_2 c_1 (\psi_j, \psi_i) = 1$

put value of c_1 as

$$[-c_2(\psi_i, \psi_j)]^2 + c_2^2 + c_2[-c_2(\psi_i, \psi_j)](\psi_i, \psi_j) + c_2[-c_2(\psi_i, \psi_j)](\psi_j, \psi_i) = 1$$

$$\cancel{c_2^2 (\psi_i, \psi_j)^2 + c_2^2 - c_2^2 (\psi_i, \psi_j)^2 -}$$

$$[-c_2(\psi_i, \psi_j)]^2 + c_2^2 + c_2\{-c_2(\psi_i, \psi_j)\}[(\psi_i, \psi_j) + (\psi_j, \psi_i)] = 1$$

$$\cancel{c_2^2 (\psi_i, \psi_j)^2} + c_2^2 - \cancel{c_2^2 (\psi_i, \psi_j)^2} - c_2^2 |(\psi_i, \psi_j)|^2 = 1$$

$$\because (\psi_i, \psi_j)(\psi_j, \psi_i) = (\psi_i, \psi_j)(\psi_i, \psi_j)^*$$
$$= |(\psi_i, \psi_j)|^2$$

so

$$c_2 = \frac{1}{\sqrt{1 - |(\psi_i, \psi_j)|^2}}$$

so

$$\psi_k = \frac{-(\psi_i, \psi_j)\psi_i}{\sqrt{1 - |(\psi_i, \psi_j)|^2}} + \frac{\psi_j}{\sqrt{1 - |(\psi_i, \psi_j)|^2}}$$

$$\psi_k = \frac{\psi_j - \psi_i (\psi_i, \psi_j)}{\sqrt{1 - |(\psi_i, \psi_j)|^2}}$$

proved

Theorem:

prove that $\langle T^n \rangle = \langle T \rangle^n$, where T is an operator applied on a wave fn ψ having λ as an eigen v.

Proof:-

$$\langle T^n \rangle = \int \psi^* T^n \psi \, d^3r$$

$$= \int \psi^* T^{n-1} (T\psi)\, d^3r$$
$$= \int \psi^* T^{n-1} (\lambda \psi)\, d^3r$$
$$= \lambda \int \psi^* T^{n-1} \psi\, d^3r$$

$$= \lambda \int \psi^* T^{n-2} (T\psi)\, d^3r$$
$$= \lambda \int \psi^* T^{n-2} (\lambda \psi)\, d^3r$$
$$= \lambda^2 \int \psi^* T^{n-2} \psi\, d^3r$$

Continuing in the same manner, we get
$$= \lambda^n \int \psi^* \psi\, d^3r = \lambda^n (1) = \lambda^n$$

R.H.S:-
$$\langle T \rangle^n = \left(\int \psi^* T \psi\, d^3r \right)^n$$
$$= \left(\int \psi^* \lambda \psi\, d^3r \right)^n = \lambda^n \left(\int \psi^* \psi\, d^3r \right)^n$$
$$= \lambda^n (1)^n = \lambda^n$$

so $\langle T^n \rangle = \langle T \rangle^n$

Simultaneous Measurability Observables-

Compatibe Observables:-

Two observables are said to be compatible if they have common set of eigen fns.

Theorem: Two operators, those have same/common set of eigenfns, are commute.

proof:-

let T_1 & T_2 be two operators having eigenvalues λ_i & μ_i respectively. And let ψ_i be a common set of eigenfns.

As $T_1 \psi_i = \lambda_i \psi_i$

$T_2 \psi_i = \mu_i \psi_i$

we find $T_1 T_2 \psi_i = T_1 (T_2 \psi_i)$

$= T_1 (\mu_i \psi_i)$

$= \mu_i (T_1 \psi_i) = \mu_i \lambda_i \psi_i$

$= \lambda_i \mu_i \psi_i$

Now

$T_2 T_1 \psi_i = T_2 (T_1 \psi_i) = T_2 (\lambda_i \psi_i) = \lambda_i (T_2 \psi_i)$

$= \lambda_i \mu_i \psi_i$

we have obtained

$T_1 T_2 = T_2 T_1$

$\Rightarrow [T_1, T_2] = 0$

$\Rightarrow$ commuted.