



p.g. sem-II, unit-I Quantum Chem.  
Ref.....

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Hermitian operators:— An operator  $\hat{A}$  is said to be Hermitian if it satisfies the following relation.

$$\int (\hat{A}\psi_i)^* \psi_j d\tau = \int \psi_i^* \hat{A}\psi_j d\tau \quad \text{--- (1)}$$

when  $\psi_i$  and  $\psi_j$  are two wave functions.

In bracket notation eqn (1) becomes.

$$\langle \hat{A}\psi_i | \psi_j \rangle = \langle \psi_i | \hat{A}\psi_j \rangle \quad \text{--- (2)}$$

Eqn (1) and (2) is obviously satisfied for ~~any~~ any real multiplication operator.

For example.

if  $\hat{A} = u$  then

$$\begin{aligned} \langle \hat{A}\psi_i | \psi_j \rangle &= \langle u\psi_i | \psi_j \rangle = \int (u\psi_i)^* \psi_j d\tau \\ &= \int \psi_i^* u \psi_j d\tau = \langle \psi_i | u\psi_j \rangle \end{aligned}$$

Thus  $A = u$  is Hermitian

It is very important to note that a quantum mechanical operator satisfies the following condition known as Hermitian condition.

if an operator  $\hat{A}$  has two eigenfunctions  $\psi$  &  $\phi$

and if,

$$\int \psi (\hat{A}\phi) d\tau = \int (\hat{A}\psi) \phi d\tau \quad \text{--- (1)}$$

when  $\psi$  and  $\phi$  are real

$$\text{or } \int \psi^* (\hat{A}\phi) d\tau = \int (\hat{A}\psi)^* \phi d\tau \quad \text{--- (2)}$$

when  $\psi$  and  $\phi$  are complex,  $\psi^*$  is the complex conjugate of  $\psi$  and  $d\tau$  is the volume element of space in which the function is defined. Then the operator  $\hat{A}$  is called Hermitian operator.