

Theorem (3)

A wavefunction which is not an eigenfunction of an operator \hat{A} can be arbitrarily expanded in a series of orthonormal functions.

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If it can be linear superposition of the orthonormal eigenfunctions of \hat{A} .

Proof \Rightarrow The proof of this theorem has not been rigorously established but it seems to be valid for Hermitian operators.

This theorem states that

$$\psi = \sum c_i \phi_i \quad (1)$$

Where ψ is an arbitrary function and ϕ_i are orthonormal functions.

They are both orthogonal and normalized.

$$\int \phi_i^* \phi_j d\tau = 0 \quad (\text{orthogonality condition}) \quad (2)$$

$$\int \phi_i^* \phi_i d\tau = 1 \quad (\text{normalization condition}) \quad (2)$$

The two conditions or criteria can be summed up by the relation

$$\int \phi_i^* \phi_j d\tau = \delta_{ij} = \begin{cases} 1, & i=j \\ 0, & i \neq j \end{cases} \quad (3)$$

Where δ_{ij} is called the Kronecker delta.

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Theorem ④

Virial Theorem \Rightarrow According to the virial theorem if the potential energy $V(x)$ of a quantum mechanical system moving in the x -direction is of the form

$$V(x) \propto x^s \quad \text{--- (1)}$$

where s is a constant, then the expectation (average) values of the kinetic energy $\langle \hat{T} \rangle$ and the expectation value of the potential energy $\langle \hat{V} \rangle$ are related by

$$\langle \hat{T} \rangle = \frac{1}{2} s \langle \hat{V} \rangle \quad \text{--- (2)}$$

Virial theorem is very important theorem in quantum mechanics and is the real test of the accuracy of the wavefunction of the quantum mechanical system (atom or molecule) obtained by the solution of the Schrödinger wave equation by the Hartree - Fock self-consistent field (SCF) method.

Theorem ⑤

Variation Theorem \Rightarrow If ψ is the approximate wave function of a quantum mechanical system described by the Hamiltonian \hat{H} , then the expectation value of the energy $\langle E \rangle$ given by the integral.

$$\langle E \rangle = \int \psi^* \hat{H} \psi d\tau \equiv \langle \psi^* | \hat{H} | \psi \rangle$$

is an upper limit to the ground state energy E_0 of the system.

$$E \geq E_0$$