

Study Notes On Variation Method



VARIATION METHOD

The approximate method based on the variation theorem is known as the Variation Method. It is a method of checking and improving the guesses in the form of trial wave functions (Ψ_{trial}) for the complex systems whose exact solution is not possible or not known.

The appropriate trial wavefunction is chosen and it is assumed to be the solution of Schrodinger equation. However, the chosen trial wavefunction may not necessarily be the eigen function of the Schrodinger equation but it must be as close as possible to the true wavefunction. The trial wavefunction is written with a few adjustable parameters, and therefore, we can calculate the energy of the system (E_a) with trial wave function.

The trial energy (E_a) corresponding to the trial wavefunction is calculated as:

$$E_a = \frac{\int \Psi_{\text{trial}}^* \cdot \hat{H}_{op} \cdot \Psi_{\text{trial}} \cdot d\tau}{\int \Psi_{\text{trial}}^* \cdot \Psi_{\text{trial}} \cdot d\tau} = \frac{\langle \Psi_{\text{trial}} | \hat{H}_{op} | \Psi_{\text{trial}} \rangle}{\langle \Psi_{\text{trial}} | \Psi_{\text{trial}} \rangle}$$

where $E_a \geq E_0$ (Exact ground state energy).

If the trial wavefunction is normalised, then the denominator of the above equation reduces to unity (condition for normalisation) and hence E_a becomes

$$E_a = \int \Psi_{\text{trial}}^* \cdot \hat{H}_{op} \cdot \Psi_{\text{trial}} \cdot d\tau = \langle \Psi_{\text{trial}} | \hat{H}_{op} | \Psi_{\text{trial}} \rangle$$

It is mandatory that under any condition, the trial energy (E_a) must always be greater or equal to the exact ground state energy (E_0).

When the trial wave function matches the true wave function then

$$E_a = E_0$$

Otherwise, trial energy corresponding to the trial wavefunction is always greater than the exact ground state energy corresponding to the true wavefunction.

So,

$$E_a > E_0$$

Therefore, by combining the two equations we get

$$E_a \geq E_0$$

However, if a number of guesses (trials) are made with corresponding trial energies (E_a) as $E_{a_1}, E_{a_2}, E_{a_3}, E_{a_4}, \dots$ etc. ; then, selection of the better trial wavefunction goes to the corresponding trial energy which follows the *two conditions*, which are:

(a) $E_a \geq E_0$

(b) If a set of trial energies follow the above condition ($E_a \geq E_0$) then further selection is done by choosing the energy closest to the E_0 (exact ground state energy).

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