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Lecture for M. Sc. Physics II Semester students

Paper-III: Quantum Mechanics

Unit-1

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PHY-III-203: Quantum Mechanics - II

Unit -1

Variation Method :-

Most of the problems in quantum mechanics can not be solved exactly, and hence need to be dealt with approximately. There are two common methods used in quantum mechanics: (i) Perturbation theory and (ii) The variation method.

The perturbation theory is useful when there is small dimensionless parameter in the problem, and the system has exact solution when small parameter is sent to zero. The system is then studied in power series expansion in the small parameter.

The variation method is useful to study the ground state, but not very useful for the study of excited states. On the other hand, it is not required that the system has a small parameter, nor that the system is solvable exactly under ~~cer~~ certain limits.

★ For determination of ground state energy E_0, for any particle:

Variation method is specially applicable for determination of lowest energy state of the particle. But, in some exceptional cases it can also be applied for determining higher energy states or excited energy states

P.T.O.

Variation method is based on fallowing concepts :-

1.) Variation method is primarily used for estimation of ground state energy ; in special cases it may be expanded to higher energy states rather than lowest energy state.

2.) It is based on the fact that the lowest value of which of the expectation value of Hamiltonian can take is ground state energy. Thus, we can say that variation method provides an upper bound to the ground state energy.

Now, Let ψ_n denotes the exact set of Eigen functions of Hamiltonian. Then we may have

$$\boxed{H\psi_n = E_n \psi_n} \qquad -(1)$$

Now, these eigen function consist of complete set of functions such that a trial function ϕ can be expanded in the terms of Eigen function as -

$$\boxed{\phi = \sum_n a_n \psi_n} \qquad -(2)$$

where, ϕ is normalized.

Expectation value of Hamiltonian can be written as

$$\boxed{\langle H \rangle = \int \psi_n^* H \psi_n \, d\tau} \qquad -(3)$$

Thus, here also we can assume that ψ_n is normalized.

Now consider the quantity E_ϕ as -

$$\boxed{E_\phi = \frac{\int \phi^* H \phi \, d\tau}{\int \phi^* \phi \, d\tau}} \quad - (4)$$

Now putting the value of eq^n (2) in eq^n (4) and applying the orthonormality Condition.

$$\boxed{E_\phi = \frac{\int (\sum_n a_n^* \psi_n^* \, H \sum_n a_n \psi_n) \, d\tau}{\int (\sum_n a_n^* \psi_n^*)(\sum_n a_n \psi_n) \, d\tau}}$$

After applying the completeness and normalization Condition [i.e, $\int \psi_n^* \psi_n d\tau = 1$], we get

$$\boxed{E_\phi = \frac{\sum_n a_n^* a_n E_n}{\sum_n a_n^* a_n}} \quad - (5)$$

Then,

$$\boxed{E_\phi = \frac{\sum_n |a_n|^2 E_n}{\sum_n |a_n|^2}}$$

[$\because a_n^*$ is complex conjugate of a_n]

Now, Subtract the ground energy state E_0 from both sides;

$$\boxed{E_\phi - E_0 = \frac{\sum_n |a_n|^2 (E_n - E_0)}{\sum_n |a_n|^2}} \quad - (6)$$

Since, E_0 is ground state energy then by definition, we can write it is smaller or equal to E_n

i.e, $E_0 \leq E_n$

and $|a_n|^2 \geq 0 \quad \forall n$

Then R.H.S. of eq^n (6) is always positive and thus L.H.S is also positive

Thus, from eqⁿ (6), we may have

$$\boxed{E\phi \geqslant E_0} \quad — (7)$$

The above equation (7) shows that the variation method provides an upper bound to the ground state energy E_0 having a suitable trail function ϕ with different parameters.

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