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PROBLEM SOLVING OF FIRST AND SECOND-ORDER STATIONARY PERTURBATION FOR NONDEGENERATE CASE USING TIME INDEPENDENT QUANTUM APPROXIMATION

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ABSTRACT

In this paper, we try to solve the stationary perturbation problem for the nondegenerate case.This case solves by using time-independent quantum approximation.Here, the Hamiltonian providing the solution of discreet eigen energy state with small and large disturbances of any quantum system.

Introduction

The Stationary perturbation theory is concerned with finding the changes in the energy levels and eigenfunction of a system when a small disturbance is applied. In such a case, the Hamiltonian can be broken up into two parts –

i. One of which is large and represents a system for which the Schrodinger equation can be solved exactly and
ii. The other part is small and can be treated as a perturbation term.

If the potential energy is disturbed by the influence of additional forces, the energy levels are shifted and for a weak perturbation, the amount of shift can be estimated in original unperturbed states are known.

Consider a physical system subjected to a perturbation which shifts the energy levels slightly, of course, the arrangement remains the same. Mathematically the effect of perturbation is to introduce additional terms in the Hamiltonian of the unperturbed system (or unchanged system). This additional term may be constant or it may be a function of both space and momentum coordinates.

In other words, the Hamiltonian H in the Schrodinger equation can be written as the sum of two parts –

i. One of these parts H^0 corresponds to the unperturbed system and
ii. Another part $H^{'}$ corresponds to the perturbation effect.

METHOD

Let us write the Schrodinger wave equation –

$$\widehat{H}\Psi = E\Psi \qquad \text{..... (1)}$$

in which Hamiltonian $\widehat{H}$ represents the operator

$$\widehat{H} = -\frac{\hbar^2}{2}\sum_i \frac{1}{m_i}\nabla_i^2 + V \qquad \text{..... (2)}$$

Let E be the eigen values of Ψ is eigen function of operator $\widehat{H}$. $\widehat{H}$ is the sum of two terms $H^0$and $H^{'}$ already defined –

$$H = H^0 + H^{'} \qquad \text{...... (3)}$$

where $H^{'}$ is small perturbation term.

Let Ψ_k^0 and E_k^0 be a particular orthonormal eigenfunction and eigenvalue of unperturbed Hamiltonian H^0, i.e.,

$$H^0\Psi_k^0 = E_k^0\Psi_k^0$$

If we consider the nondegenerate system for which there is one eigenfunction corresponding to each eigenvalue. In the stationary system, the Hamiltonian H does not depend upon time and it is possible to expend H in terms of some parameter λ yielding the expression

$$H = H^0 + \lambda H^{'} + \lambda^2 H^{''} + \cdots \qquad \text{...... (4)}$$

in which λ has been chosen in such a way that equation (1) for $\lambda = 0$ reduces to the form

$$H^0\Psi^0 - E^0\Psi^0 = 0 \qquad \text{...... (5)}$$

It is to be remembered that this is one eigenfunction Ψ and energy level E^0corresponding to operator H^0 . Equation (5) can be directly solved. This equitation is said to be the "wave equation of unperturbed system" which the terms $\lambda H^{'} + \lambda^2 H^{''} + \cdots$ are called the perturbed terms.

The unperturbed equation (5) has a solution$\Psi^0, \Psi_1^0, \Psi_2^0, \ldots \Psi_k^0, \ldots$ called the unperturbed eigenfunctions and corresponding eigenvalues are$E_0^0, E_1^0, E_2^0, \ldots\ldots\ E_k^0, \ldots..$

The function Ψ_k^0 form a complete set, i.e., they satisfy the condition

$$\int \Psi_i^{0*}\Psi_j d\tau = \delta_{ij} \qquad \text{...... (6)}$$

where $\delta_{ij}$is Kronecker delta symbol defined as$\delta_{ij} = \begin{cases} 0 \text{ for } i \neq j \\ 1 \text{ for } i = j \end{cases}$(Jafarpour, M., & Afshar, D., 2001).

Now let us consider the effect of perturbation. The application of perturbation does not cause large change hence the energy values and wavefunctions for the perturbed system will be near to those for the unperturbed system. We can expand the energy E and the wave function Ψ for the perturbed system in terms ofλ, so

$$\Psi_k = \Psi_k^0 + \lambda\Psi_k^{'} + \lambda^2\Psi_k^{''} + \cdots \qquad ....(7)$$

$$E_k = E_k^0 + \lambda E_k^{'} + \lambda^2 E_k^{''} + \ldots \qquad ....(8)$$

If the perturbation is small, the terms of the series (7) and (8) will become rapidly smaller i.e., the series will be convergent.

Now substituting (6) and (7) and (8) in equation (1), we get

$$\left(H^0 + \lambda H^{'} + \lambda^2 H^{''} + \cdots\right)\left(\Psi_k^0 + \lambda\Psi_k^{'} + \lambda^2\Psi_k^{''} + \cdots\right) = \left(E_k^0 + \lambda E_k^{'} + \lambda^2 E_k^{''} + \cdots\right)\left(\Psi_k^0 + \lambda\Psi_k^{'} + \lambda^2\Psi_k^{''} + \cdots\right)$$

On collecting the coefficient of like power λ.

$$\left(H^0\Psi_k^0 - E_k^0\Psi_k^0\right) + \left(H^0\Psi_k^{'} + H^{'}\Psi_k^0 - E_k^0\Psi_k^{'} - E_k^{'}\Psi_k^0\right)\lambda + \left(H^0\Psi_k^{''} + H^{'}\Psi_k^{'} + H^{''}\Psi_k^0 - E_k^0\Psi_k^{''} - E_k^{'}\Psi_k^{'} - E_k^{''}\Psi_k^0\right)\lambda^2 + \cdots = 0 \ldots (9)$$

In this series is properly convergent i.e., equal to zero all possible values of λ, then coefficients of various powers of λ must vanish separately. These equations will have successfully higher orders of the perturbation. The coefficient of λ^0 gives (Griffiths, D. J., 2005).

$$\left(H^0 - E_k^0\right)\Psi_k^0 = 0 \qquad \ldots\ldots (10a)$$

The coefficient of λ gives

$$\left(H^0\Psi_k^{'} + H^{'}\Psi_k^0 - E_k^0\Psi_k^{'} - E_k^{'}\Psi_k^0\right) = 0$$

$$\left(H^0 - E_k^0\right)\Psi_k^{'} + \left(H^{'} - E_k^{'}\right)\Psi_k^0 = 0 \qquad \ldots\ldots (10b)$$

The coefficient of λ^2 gives

$$\left(H^0\Psi_k^{''} + H^{'}\Psi_k^{'} + H^{''}\Psi_k^0 - E_k^0\Psi_k^{''} - E_k^{'}\Psi_k^{'} - E_k^{''}\Psi_k^0\right) = 0$$

$$\left(H^0 - E_k^0\right)\Psi_k^{''} + \left(H^{'} - E_k^{'}\right)\Psi_k^{'} + \left(H^{''} - E_k^{''}\right)\Psi_k^0 = 0 \qquad \ldots\ldots (10c)$$

Similarly, the coefficient of λ^3 gives

$$\left(H^0 - E_k^0\right)\Psi_k^{'''} + \left(H^{'} - E_k^{'}\right)\Psi_k^{''} + \left(H^{''} - E_k^{''}\right)\Psi_k^{'} + \left(H^{'''} - E_k^{'''}\right)\Psi_k^0 = 0 \qquad \ldots\ldots (10d)$$

But if we limit the total Hamiltonian H upto $\lambda H'$, i.e., if we put $H = H^0 + \lambda H'$, then equations (10) will be modified as

$$\left(H^0 - E_k^0\right)\Psi_k^0 = 0 \qquad \ldots\ldots (11a)$$

$$\left(H^0 - E_k^0\right)\Psi_k^{'} + \left(H^{'} - E_k^{'}\right)\Psi_k^0 = 0 \qquad \ldots\ldots (11b)$$

$$\left(H^0 - E_k^0\right)\Psi_k^{''} + \left(H^{'} - E_k^{'}\right)\Psi_k^{'} - E_k^{''}\Psi_k^0 = 0 \qquad \ldots\ldots (11c)$$

$$\left(H^0 - E_k^0\right)\Psi_k^{'''} + \left(H^{'} - E_k^{'}\right)\Psi_k^{''} - E_k^{''}\Psi_k^{'} - E_k^{'''}\Psi_k^0 = 0 \qquad \ldots\ldots (11d)$$

First order perturbation

From equation (11b),

$$\left(H^0 - E_k^0\right)\Psi_k^{'} + \left(H^{'} - E_k^{'}\right)\Psi_k^0 = 0$$

To solve this equation we use expansion theorem. As perturbation is very small, the deviations from the unperturbed state are small, therefore the first-order perturbation correction function $\Psi_k^{'}$ can be expended in terms of unperturbed functions $\Psi_1^0, \Psi_2^0, \ldots, \Psi_l^0, \ldots$, since Ψ_l^0 from a normalized orthonormal set (Atalla, N., &Sgard, F. 2015).

Hence, we write

$\Psi_k^{'} = \sum_{l=0}^{\infty} a_l \Psi_l^0$ ……. (12)

Substituting $\Psi_k^{'}$from (12) in (11b), we get

$$\left(H^0 - E_k^0\right)\sum_{l=0}^{\infty} a_l \Psi_l^0 + \left(H^{'} - E_k^{'}\right)\Psi_k^0 = 0$$

$$\sum_{l=0}^{\infty} a_l H^0 \Psi_l^0 - \sum_{l=0}^{\infty} a_l E_k^0 \Psi_l^0 + \left(H^{'} - E_k^{'}\right)\Psi_k^0 = 0$$

Using $H^0\Psi_l^0 = E_l^0\Psi_l^0$, we get

$$\sum_{l=0}^{\infty} a_l E_l^0 \Psi_l^0 - \sum_{l=0}^{\infty} a_l E_k^0 \Psi_l^0 + \left(H^{'} - E_k^{'}\right)\Psi_k^0 = 0$$

$$\sum_{l=0}^{\infty} a_l \left(E_l^0 - E_k^0\right)\Psi_l^0 + \left(H^{'} - E_k^{'}\right)\Psi_k^0 = 0$$

$$\sum_{l=0}^{\infty} a_l \left(E_l^0 - E_k^0\right)\Psi_l^0 = -\left(H^{'} - E_k^{'}\right)\Psi_k^0$$

$\sum_{l=0}^{\infty} a_l \left(E_l^0 - E_k^0\right)\Psi_l^0 = \left(E_k^{'} - H^{'}\right)\Psi_k^0$ ……. (13)

Multiplying above equation by $\Psi_k^{0*}$and integrating over configuration space, we get

$\sum_{l=0}^{\infty} a_l \left(E_l^0 - E_k^0\right) \int \Psi_l^0 \Psi_k^{0*} d\tau = \int \Psi_k^{0*} \left(E_k^{'} - H^{'}\right)\Psi_k^0 \, d\tau$(Al-shara, et. al.,2011).

Using the condition of orthonormalization, we get

$$\int \Psi_l^0 \Psi_k^{0*} d\tau = \delta_{ij} = \begin{cases} 0 \text{ for } i \neq j \\ 1 \text{ for } i = j \end{cases}$$

We get,

$$\sum_{l=0}^{\infty} a_l \left(E_l^0 - E_k^0\right)\delta_{ml} = \int \Psi_k^{0*} E_k^{'} \Psi_k^0 d\tau - \int \Psi_k^{0*} H^{'} \Psi_k^0 d\tau$$

$$= E_k^{'} \delta_{mk} - \int \Psi_k^{0*} H^{'} \Psi_k^0 d\tau$$

Using the notations

$$\int \Psi_k^{0*} H^{'} \Psi_k^0 d\tau = < m \middle| H^{'} \middle| k >$$

Therefore

$\sum_{l=0}^{\infty} a_l\left(E_l^0 - E_k^0\right)\delta_{ml} = E_k^{'}\delta_{mk} - < m\left|H^{'}\right|k >$……. (14)

Setting $m = k$ in equation (14), we observe that

$$\sum_{l=0}^{\infty} a_l\left(E_l^0 - E_k^0\right)\delta_{kl} = 0 \text{ always,}$$

Since$l = k, E_l^0 - E_l^0 = 0$ and for $l \neq k$, $\delta_{kl} = 0$ so that, we get

$$0 = E_k^{'} - < km\left|H^{'}\right|k >$$

Or$E_k^{'} = < km\left|H^{'}\right|k > = \int \Psi_k^{0*} H^{'} \Psi_k^0 d\tau$ …….. (15)

This expression gives first-order perturbation energy correction. Accordingly, the "first-order perturbation energy correction for a nondegenerate system is just the expectation value of first-order perturbation Hamiltonian (H′)over the unperturbed state of the system."

Second-Order Perturbation

The second-order perturbation equation (11c)

$$\left(H^0 - E_k^0\right)\Psi_k^{''} + \left(H^{'} - E_k^{'}\right)\Psi_k^{'} - E_k^{''}\Psi_k^0 = 0$$

Expanding second-order wave function $\Psi_k^{''}$ as a linear combination of unperturbed orthonormal wave functions Ψ_m^0 by expansions theorem, i.e.,

$\Psi_k^{''} = \sum_m b_m \Psi_m^0$ …….. (16)

Substituting

$$\Psi_k^{'} = \sum_l{}^{'} \frac{< l\left|H^{'}\right| k >}{E_k^0 - E_l^0}\Psi_l^0 \,;\; \Psi_k^{''} = \sum_m b_m \Psi_m^0$$

and $E_k^{'} = < l\left|H^{'}\right| k >$ in equation (11c); we get

$$\left(H^0 - E_k^0\right)\sum_m b_m \Psi_m^0 + \left(H^{'} - < l\left|H^{'}\right| k >\right)\sum_l{}^{'} \frac{< l\left|H^{'}\right| k >}{E_k^0 - E_l^0}\Psi_l^0 - E_k^{''}\Psi_k^0 = 0$$

$$H^0\sum_m b_m \Psi_m^0 - E_k^0\sum_m b_m \Psi_m^0 + \left(H^{'} - < l\left|H^{'}\right| k >\right)\sum_l{}^{'} \frac{< l\left|H^{'}\right| k >}{E_k^0 - E_l^0}\Psi_l^0 - E_k^{''}\Psi_k^0 = 0$$

Using unperturbed Schrodinger equation $H^0\Psi_m^0 = E_m^0\Psi_m^0$, we get

$$\sum_m b_m H^0\Psi_m^0 - \sum_m b_m E_k^0\Psi_m^0 + \left(H^{'} - < l\left|H^{'}\right| k >\right)\sum_l{}^{'} \frac{< l\left|H^{'}\right| k >}{E_k^0 - E_l^0}\Psi_l^0 - E_k^{''}\Psi_k^0 = 0$$

$$\sum_m b_m E_m^0\Psi_m^0 - \sum_m b_m E_k^0\Psi_m^0 + \left(H^{'} - < l\left|H^{'}\right| k >\right)\sum_l{}^{'} \frac{< l\left|H^{'}\right| k >}{E_k^0 - E_l^0}\Psi_l^0 - E_k^{''}\Psi_k^0 = 0$$

$$\sum_m b_m \left(E_m^0 - E_k^0\right)\Psi_m^0 + \left(H' - < l \left|H'\right| k >\right) \sum\nolimits_l' \frac{< l \left|H'\right| k >}{E_k^0 - E_l^0} \Psi_l^0 - E_k'' \Psi_k^0 = 0$$

Multiplying by $\Psi_n^{0*}$and integrating overall space, we get

$\sum_m b_m \left(E_m^0 - E_k^0\right) \int \Psi_n^{0*}\Psi_m^0 \, d\tau + \int \left(H' - < l \left|H'\right| k >\right) \sum_l' \frac{< l \left|H'\right| k >}{E_k^0 - E_l^0} \Psi_n^{0*}\Psi_l^0 \, d\tau - E_k'' \int \Psi_n^{0*}\Psi_k^0 d\tau = 0$ (Adelakun, A. O., & Dele, A. D., 2014).

Use the orthonormal property of unperturbed wave function, we get

$\sum_m b_m \left(E_m^0 - E_k^0\right)\delta_{nm} + \sum_l' \frac{< l \left|H'\right| k >< n \left|H'\right| l >}{E_k^0 - E_l^0} - \sum_l' \frac{< k \left|H'\right| k >< l \left|H'\right| k >}{E_k^0 - E_l^0} \delta_{nl} - E_k'' \delta_{nk} = 0$ ……. (17)

Setting $n = k$ in equation (17), we get

$\sum_m b_m \left(E_m^0 - E_k^0\right)\delta_{km} + \sum_l' \frac{< l \left|H'\right| k >< k \left|H'\right| l >}{E_k^0 - E_l^0} - \sum_l' \frac{< k \left|H'\right| k >< l \left|H'\right| k >}{E_k^0 - E_l^0} \delta_{kl} - E_k'' \delta_{kk} = 0$ …….. (18)

As $\delta_{kk} = 1$ and $\sum_m b_m \left(E_m^0 - E_k^0\right)\delta_{km} = 0$ for all values of m, equation (18) gives

$E_k'' = \sum_l' \frac{< l \left|H'\right| k >< k \left|H'\right| l >}{E_k^0 - E_l^0} - \sum_l' \frac{< k \left|H'\right| k >< l \left|H'\right| k >}{E_k^0 - E_l^0} \delta_{kl}$ ……. (19)

Considering the second term in equation (19), we note that this term is zero since $\delta_{kl} = 0$ for all values of l expected for $l = k$ and this term is not included in the summation. Then equation (19) gives

$$E_k'' = \sum\nolimits_l' \frac{< l \left|H'\right| k >< k \left|H'\right| l >}{E_k^0 - E_l^0}$$

If we assume that H' is a Hermitian operator, we may write

$E_k'' = \sum_l' \frac{\left|< l \left|H'\right| k >\right|^2}{E_k^0 - E_l^0}$ ……. (20)

This equation gives second-order energy correction term E_k''. The prime on summation reminds the omission of the term $l = k$ in the summation.

RESULT DISCUSSION AND CONCLUSION

Successfully probmem solving by time-independent approximation method. Even though limited results of this paper are probably either new or appear in a new framework, the main attention of this study is on one side the incorporated and consistent formulation of stationary perturbation theory in terms of the first and second-order time-independent approximation method. Exactly, find the first and second-order degenerate case solution.

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