PERTURBATION

THEORY

MSC 201

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Introduction : If the potential system of the real world deviates from the ideal system and amount of deviation can be identified, then we will use perturbation theory to find the eigen functions and eigen values of the hamiltonian corresponding to the potential of the real world.

There are two types of perturbation theory

i) Time Dependent Perturbation theory.

ii) Time Independent Perturbation theory.

Time Independent Perturbation Theory

If the amount of deviation of the real systems from the ideal systems is time independent and very small. The change in the energy eigen function and energy eigen values w.r.t the ideal system is small due to the deviation.

Total Hamiltonian of a system -

$$\hat{H} = \hat{H}_0 + \hat{H}_P \quad -(1)$$

where $\hat{H}$ - Perturbed hamiltonian of real system.
$\hat{H}_0$ - Unperturbed hamiltonian of Ideal system
$\hat{H}_P$ - Perturbed hamiltonian of Ideal system.

where $\hat{H}_P = \lambda H'$. $\quad -(2)$

where λ is perturbed parameter and is v. small $(\lambda << 1)$.

For unperturbed Hamiltonian, Eigen value eq -

$$H_0 |\phi_n^{(0)}\rangle = E_n^{(0)} \cdot |\phi_n^{(0)}\rangle \quad -(3)$$

Here $|\phi_n^{(0)}\rangle$ is unperturbed eigen state &
$E_n^{(0)}$ is non-degenerate unperturbed energy

Here, we are taking non-degenerate case.

$$\hat{H} |\phi_n\rangle = E_n |\phi_n\rangle \quad -(4)$$

where $\hat{H}$ is perturbed hamiltonian
E_n is perturbed Energy

Now, the energy-eigen functions and eigen-values of the perturbed hamiltonian is written in the power series expansion of λ.

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^{(2)} E_n^{(2)} + \cdots \quad -(5)$$

$$|\phi_n\rangle = |\phi_n^{(0)}\rangle + \lambda|\phi_n^{(1)}\rangle + \lambda^{(2)}|\phi_n^{(2)}\rangle + \cdots \quad -(6)$$

Here order shows order of correction.

By putting the values of E_n & $|\phi_n\rangle$ from eq (5) & (6) in eq (4) we get

$$\hat{H}\left[|\phi_n^{(0)}\rangle + \lambda|\phi_n^{(1)}\rangle + \lambda^{(2)}|\phi_n^{(2)}\rangle + \cdots\right] = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^{(2)} E_n^{(2)} + \cdots$$
$$\left[|\phi_n^{(0)}\rangle + \lambda|\phi_n^{(1)}\rangle + \lambda^{(2)}|\phi_n^{(2)}\rangle + \cdots\right]$$

Now, put the value of $\hat{H}$ from eq (1) and using eq (2) we get

$$[\hat{H}_0 + \lambda\hat{H}']\left[|\phi_n^{(0)}\rangle + \lambda|\phi_n^{(1)}\rangle + \lambda^{(2)}|\phi_n^{(2)}\rangle + \cdots\right]$$
$$= \left[E_n^{(0)} + \lambda E_n^{(1)} + \lambda^{(2)} E_n^{(2)} + \cdots\right]\left[|\phi_n^{(0)}\rangle + \lambda|\phi_n^{(1)}\rangle + \lambda^{(2)}|\phi_n^{(2)}\rangle + \cdots\right]$$

Now, comparing the coefficients of λ both the sides

comparing the coeff of λ^0 we get

$$H_0|\phi_n^{(0)}\rangle = E_n^{(0)}|\phi_n^{(0)}\rangle \quad -(7)$$

comparing the coefficient of $\lambda^{(1)}$ we get -

$$H_0|\phi_n^{(1)}\rangle + H'|\phi_n^{(0)}\rangle = E_n^{(0)}|\phi_n^{(1)}\rangle + E_n^{(1)}|\phi_n^{(0)}\rangle \quad -(8)$$

Comparing the coefficient of $\lambda^{(2)}$ we get -

$$H_0|\phi_n^{(2)}\rangle + H'|\phi_n^{(1)}\rangle = E_n^{(0)}|\phi_n^{(2)}\rangle + E_n^{(1)}|\phi_n^{(1)}\rangle + E_n^{(2)}|\phi_n^{(0)}\rangle$$
$$-(9)$$

Neglecting higher powers of λ, i.e. $\lambda^3, \lambda^4, \ldots$ and so on. and using these properties-

$$\left.\begin{aligned} \langle\phi_n|\phi_n\rangle &= 1 \\ \langle\phi_n|\phi_n^{(1)}\rangle &= 0 \\ \langle\phi_n^{(0)}|\phi_n^{(1)}\rangle &= 0 \end{aligned}\right\} \quad (10)$$

From eq (8) - Multiply by hermitian adjoint of $|\phi_n^{(0)}\rangle$ both the sides, we get -

$$\langle \phi_n^{(0)}|H_0|\phi_n^{(1)}\rangle + \langle \phi_n^{(0)}|H'|\phi_n^{(0)}\rangle = \langle \phi_n^{(0)}|E_n^{(0)}|\phi_n^{(1)}\rangle + \langle \phi_n^{(0)}|E_n^{(1)}|\phi_n^{(0)}\rangle$$

Using eq (10) we get -

$$\langle \phi_n^{(0)}|H'|\phi_n^{(0)}\rangle = \langle \phi_n^{(0)}|E_n^{(1)}|\phi_n^{(0)}\rangle$$

$$\langle \phi_n^{(0)}|H'|\phi_n^{(0)}\rangle = E_n^{(1)}\langle \phi_n^{(0)}|\phi_n^{(0)}\rangle$$

$$\therefore \boxed{E_n^{(1)} = \langle \phi_n^{(0)}|H'|\phi_n^{(0)}\rangle} \quad \text{— (A)}$$

This is the I order correction in energy i.e. the expectation value of perturbed hamiltonian over unperturbed state.

Calculation of I order correction in wave function $|\phi_n^{(1)}\rangle$ -

By using completeness eq of projection operator

$$|\phi_n^{(1)}\rangle = \hat{I}\,|\phi_n^{(1)}\rangle$$

$$|\phi_n^{(1)}\rangle = \Big(\sum_{\substack{m \\ m\neq n}} |\phi_m^{(0)}\rangle\langle \phi_m^{(0)}|\Big)|\phi_n^{(1)}\rangle$$

Multiplying by $\langle \phi_m^{(0)}|$ in eq (8)

$$\langle \phi_m^{(0)}|H_0|\phi_n^{(1)}\rangle + \langle \phi_m^{(0)}|H'|\phi_n^{(0)}\rangle = \langle \phi_m^{(0)}|E_n^{(0)}|\phi_n^{(1)}\rangle + E_n^{(1)}\langle \phi_m^{(0)}|\phi_n^{(0)}\rangle$$

$$E_m^{(0)}\langle \phi_m^{(0)}|\phi_n^{(1)}\rangle + \langle \phi_m^{(0)}|H'|\phi_n^{(0)}\rangle = E_n^{(0)}\langle \phi_m^{(0)}|\phi_n^{(1)}\rangle$$

$$\langle \phi_m^{(0)}|H'|\phi_n^{(0)}\rangle = E_n^{(0)} - E_m^{(0)}\,[\langle \phi_m^{(0)}|\phi_n^{(1)}\rangle$$

$$\therefore \frac{\langle \phi_m^{(0)}|H'|\phi_n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} = \langle \phi_m^{(0)}|\phi_n^{(1)}\rangle$$

$$\boxed{|\phi_n^{(1)}\rangle = \sum_{m\neq n} \frac{\langle \phi_m^{(0)}|H'|\phi_n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}}|\phi_m^{(0)}\rangle} \quad \text{— (B)}$$

defined by potential $V(x)$ given by.

$$V(x) = \begin{cases} 0 & 0<x<a, \; 0<y<a \\ \infty & \text{otherwise} \end{cases}$$

its normalized eigen functions are-

$$\psi_{n_x,n_y}(x,y) = \frac{2}{a} \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{a}\right)$$

where $n_x, n_y = 1, 2, 3, \ldots$

If a perturbation

$$H' = \begin{cases} V_0 & 0<x<a/2, \; 0<y<a/2 \\ 0 & \text{otherwise} \end{cases}$$ is applied

find out the I order correction in energy.

Solution

$\because$ we know

$$E_n^{(1)} = \langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle$$

$$\therefore E_{n_x,n_y}^{(1)} = \langle \psi_{n_x,n_y} | H' | \psi_{n_x,n_y} \rangle$$

$$E_{n_x,n_y}^{(1)} = \int_0^{a/2}\int_0^{a/2} \left(\frac{2}{a}\right) \sin\left(\frac{n_x \pi x}{a}\right) \cdot \sin\frac{n_y \pi y}{a} \cdot V_0 \cdot \left(\frac{2}{a}\right) \sin\left(\frac{n_x \pi x}{a}\right) \cdot \sin\frac{n_y \pi y}{a}\, dx\, dy$$

$$= V_0 \int_0^{a/2} \left(\frac{2}{a}\right) \sin^2\left(\frac{n_x \pi x}{a}\right) dx \int_0^{a/2} \left(\frac{2}{a}\right) \sin^2 \frac{n_y \pi y}{a}\, dy$$

$$= \frac{4V_0}{a^2}\left[\int_0^{a/2}\left(\frac{1-\cos\frac{2n_x \pi x}{a}}{2}\right) dx \cdot \int_0^{a/2}\left(\frac{1-\cos 2n_y \pi y/a}{2}\right) dy\right]$$

$$= \frac{\cancel{4}}{\cancel{a^2}} V_0 \left[\left(\frac{\cancel{a}}{\cancel{4}}\right) \cdot \left(\frac{\cancel{a}}{4}\right)\right]$$

$$= \frac{V_0}{4}$$

Ans


THANK
YOU
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