

Time independent Perturbation

Ananth

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Consider a Hamiltonian

$$\hat{H} = \hat{H}_0 + \lambda \hat{H}' \quad (1)$$

where H_0 is a simple solvable Hamiltonian e.g., harmonic oscillator or H2 atom. H' is a small term added to the main Hamiltonian.

$$\lambda = 0 \rightarrow 1$$

is an on off switch of perturbation H'

$$\lambda = 0 \Rightarrow H |\chi_n\rangle = H_0 |\chi_n\rangle = E_n^0 |\chi_n\rangle$$

$H_0 |\chi_n\rangle = E_n^0 |\chi_n\rangle$ is the energy Eigen-value problem of the undisturbed Hamiltonian with a state vectors $|\chi_n\rangle$. The superscript 0 in the eigen value is just a superficial reminder to us it is an undisturbed Hamiltonian's eigen value Let $|\psi_n\rangle$ be the solution when $\lambda = 1$ or any finite value.

$$\hat{H} |\psi_n\rangle = E_n |\psi_n\rangle$$

upper index order of perturbation. Lower index quantum numbers or state indices of H_0

Where $|\psi_n\rangle$ is the possible exact solution. Since we do not know the exact solution we can write both the state vector $|\psi_n\rangle$ and Energy Eigen value E_N as an expansion in powers of λ

$$\hat{X}_n |\psi_n\rangle = |\chi_n\rangle + (\lambda |\phi_n^1\rangle + \lambda^2 |\phi_n^2\rangle + \lambda^3 |\phi_n^3\rangle) + \dots \quad (2)$$

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots \quad (3)$$

λ is just an index to the power. $n = 0$ is simply no perturbation. The order $n = 1$ implies you take all terms up to 1. The indices in the subscript correspond to quantum number and the superscript to the perturbation order.

$$\hat{H} |\psi_n\rangle = (H_0 + \lambda H') (|\chi_n\rangle + \lambda |\phi_n^1\rangle + \lambda^2 |\phi_n^2\rangle + \lambda^3 |\phi_n^3\rangle + \dots)$$

Assume there some eigen values for both H and H' some may be trivially zero Group all the terms with

same power of λ

e.g. $\lambda = 0$ is simply $H_0 |\psi_n^0\rangle = E_n^0 |\psi_n^0\rangle$ rewrite as

$$H_0 |\psi_n^0\rangle - E_n^0 |\psi_n^0\rangle = 0$$

Take $\lambda = 1$

$$H_0 |\phi_n^1\rangle + H' |\chi_n\rangle$$

If you multiply this by a bra-vector $\langle\chi_n|$

$$E_n^0 \cancel{\langle\chi_n|} |\phi_n^1\rangle + \langle\chi_n| H' |\chi_n\rangle$$

you can write

$$\Delta E^1 = \langle\chi_n| H' |\chi_n\rangle$$

the correction to E_n^0

$$(H_0 + \lambda H')(|\chi_n^0\rangle + \lambda |\phi_n^1\rangle + \lambda^2 |\phi_n^2\rangle + \lambda^3 |\phi_n^3\rangle - (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots)(|\chi_n\rangle + \lambda |\phi_n^1\rangle + \lambda^2 |\phi_n^2\rangle + \lambda^3 |\phi_n^3\rangle)$$

Now do a book keeping to keep all similar order terms in above equation.

$$(H_0 - E_n^0) |\chi_n\rangle = 0 \text{ unperturbed}$$

$$(H_0 - E_n^0) |\phi_n^1\rangle + E_n^1 |\chi_n\rangle = \hat{H}' |\chi_n\rangle \text{ 1st order}$$

$$(H_0 - E_n^0) |\phi_n^2\rangle + E_n^1 |\phi_n^1\rangle + E_n^2 |\chi_n\rangle = \hat{H}' |\phi_n^1\rangle \text{ 2nd order (5)}$$

The idea of perturbation is all terms like $|\phi_n^i\rangle$ are all orthogonal to $|\chi_n\rangle$. If $|\chi_n\rangle$ is a solution of H_0 it is a subset of all other solutions e.g $|\chi_{n+1}\rangle$ being another state. What does a small perturbation do it mixes other states e.g $|\chi_{n+1}\rangle$ or $|\chi_m\rangle$ as long as the

index is not same as n . If the index is same as n then there is no effect of perturbation. To find the wave function e.g for 1st order take any state $|\chi_m\rangle$ of H_0 where $m \neq n$ and project it on eqn 6 1st order terms

$$\langle \chi_m | H' | \chi_n \rangle = (E_n^0 - E_m^0) \langle \chi_m | \phi_n^1 \rangle$$

Now sum over all $m \neq n$ states to get the linear combination.

$$|\phi_n^1\rangle = \sum_{m \neq n} \frac{\langle \chi_m | H' | \chi_n \rangle}{(E_n^0 - E_m^0)} |\chi_m\rangle$$