12/2/98

Lecture #37 Degenerate Perturbation Theory

Last time expanded wave function and energy in a power series in powers of small perturbation H'

1st order: $H^0 \psi_n^1 + H' \psi_n^0 = E_n^0 \psi_n^1 + E_n^1 \psi_n^0$ (A)

2nd order: $H^0 \psi_n^2 + H' \psi_n^1 = E_n^0 \psi_n^2 + E_n^1 \psi_n^1 + E_n^2 \psi_n^0$ (B)

1st order Energy $\quad E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle$

1st order Wave func $\quad \psi_n^1 = \sum_{m \neq n} \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0} \psi_m^0$

Assumes <u>non degenerate</u> $E_m^0 \neq E_n^0$ for $m \neq n$

<u>2nd order Energy</u>

Take inner product of (B) with $\langle \psi_n^0 |$

$$\underbrace{\langle \psi_n^0 | H^0 \psi_n^2 \rangle}_{= \cancel{\langle \psi_n^0 | E_n^0 \psi_n^2 \rangle}} + \langle \psi_n^0 | H' | \psi_n^1 \rangle = \cancel{E_n^0 \langle \psi_n^0 | \psi_n^2 \rangle} + E_n^1 \langle \psi_n^0 | \psi_n^1 \rangle + E_n^2 \langle \psi_n^0 | \psi_n^0 \rangle$$

$\langle \psi_n^0 | \psi_n^1 \rangle = 0$ since no $|\psi_n^0\rangle$ in $|\psi_n^1\rangle$

$$E_n^2 = \langle \psi_n^0 | H' | \psi_n^1 \rangle$$

$$= \sum_{n \neq m} \langle \psi_n^0 | H' | \psi_m^0 \rangle \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0}$$

$$\boxed{E_n^2 = \sum_{n \neq m} \frac{|\langle \psi_n^0 | H' | \psi_m^0 \rangle|^2}{E_n^0 - E_m^0}}$$

- Valid for any state n.
- For ground state $n=0$ say

$$E_m^0 > E_0^0 \quad \text{for all } m$$

$\Rightarrow$ 2^{nd} order shift in energy of ground state is always negative

$$E_0^2 = \sum_{m \neq 0} \frac{|\langle \psi_0^0 | H' | \psi_m^0 \rangle|^2}{-(E_m^0 - E_0^0)} \leq 0$$

Degenerate perturbation theory

- What to do if $E_m^0 = E_n^0$ for $m \neq n$?
- We expect only small changes in the wave function if H' is small.

That is ψ_n^1 is of order H'
However if there are degeneracies this is not true.

Two fold degeneracy

$$H^0 \psi_a^0 = E^0 \psi_a^0 \quad \text{and} \quad H^0 \psi_b^0 = E^0 \psi_b^0$$

with

$$\langle \psi_a^0 | \psi_b^0 \rangle = 0$$

Any combination

$$\psi^0 = \alpha \psi_a^0 + \beta \psi_b^0$$

is still an eigenstate of H^0

$$H^0 \psi^0 = E^0 \psi^0$$

Typically H' will break this degeneracy. Even a very small H' can lead to large changes in α, β because they are not constrained without H'.

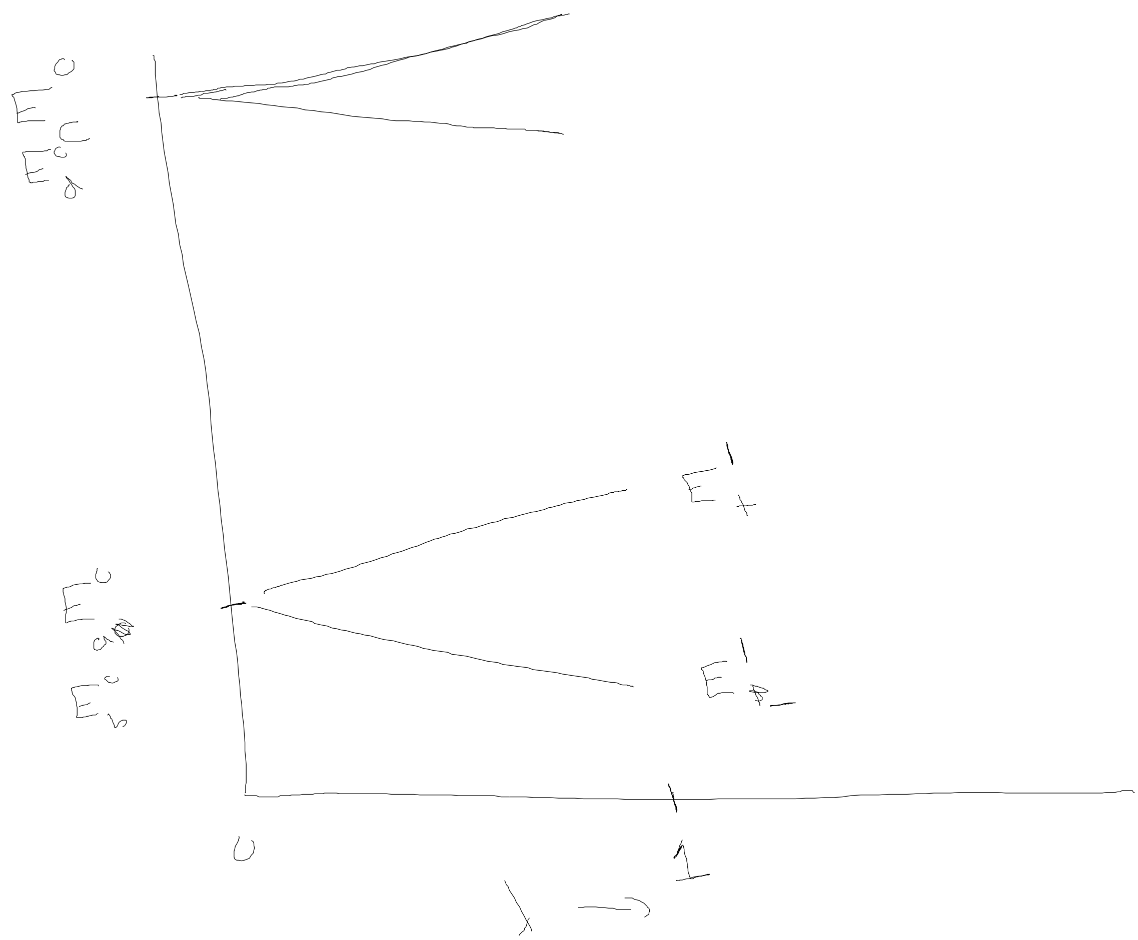
Rule: Diagonalize the perturbation in the degenerate subspace to find the best α, β

Define

$$W_{ij} = \langle \psi_i^0 | H' | \psi_j^0 \rangle$$

$$\begin{bmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{bmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E^1 \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$E'_{\pm} = \frac{1}{2}\left[W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{ab}|^2}\right]$$



Note if you diagonalize $H^0 + H'$ in whole space you solve problem exactly

Here only diagonalize in small subspace.