Lecture 6

Time-independent perturbation theory

Given a Hamiltonian

$$H = H^0 + \lambda H'$$ (e.g. H atom in a small electric field)

Solutions to H^0 are known:

$$H^0 \psi_n^0 = E_n^0 \psi_n^0 \quad ; \quad \langle \psi_n^0 | \psi_{n'}^0 \rangle = \delta_{nn'}$$

$\{\psi_n^0\}$ form a complete set in the Hilbert space of the system,
H' is the perturbing Hamiltonian and
λ is a small number (irrelevant in the end, just a counting device)

Find the approximate eigensolutions of H.
We use perturbation theory:
Let us assume E_n are nondegenerate

Write

$$(1) \quad \begin{cases} \psi_n = \psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots \\ E_n = \underbrace{E_n^0}_{\text{zero-order correction}} + \lambda \underbrace{E_n^1}_{\text{1st-order correction}} + \lambda^2 \underbrace{E_n^2}_{\text{2nd-order correction}} + \dots \end{cases}$$

Put (1) into $H\psi_n = E_n\psi_n$ (note n is assumed to be the same as the unperturbed case)

$$(H^0 + \lambda H^1)\left[\psi_n^0 + \lambda\psi_n^1 + \lambda^2\psi_n^2 + \dots\right] =$$
$$= (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots)\left[\psi_n^0 + \lambda\psi_n^1 + \lambda^2\psi_n^2 + \dots\right]$$

$$\Downarrow$$

$$H^0\psi_n^0 + \lambda(H^0\psi_n^1 + H^1\psi_n^0) + \lambda^2(H^0\psi_n^2 + H^1\psi_n^1) + \dots$$
$$= E_n^0\psi_n^0 + \lambda(E_n^0\psi_n^1 + E_n^1\psi_n^0) + \lambda^2(E_n^0\psi_n^2 +$$
$$+ E_n^1\psi_n^1 + E_n^2\psi_n^0) + \dots$$

zero order : $H^0\psi_n^0 = E_n^0\psi_n^0$

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

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

Solve up to first order:

multiply (1) by $\langle \psi_n^0 |$ and integrate

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

$$(H^0)^+ = H^0 \quad ; \quad \langle \psi_n^0 | \psi_n^0 \rangle = 1$$

$$\Downarrow$$

$$\langle \psi_n^0 | H^0 \psi_n^1 \rangle = \langle H^0 \psi_n^0 | \psi_n^1 \rangle = E_n^0 \langle \psi_0^n | \psi_n^1 \rangle$$

$$\Downarrow$$

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

$$E = E_0 + \underbrace{\langle \psi_n^0 | H^1 | \psi_n^0 \rangle}_{\substack{\text{expectation} \\ \text{value of the} \\ \text{perturbation on} \\ \text{the unperturbed} \\ \text{state}}} + \ldots$$

First-order perturbation to the w.f.

rewrite (1) as $\left(H^0 - E_n^0\right)\psi_n^1 = -\left(H^1 - E_n^1\right)\psi_n^0$

since $\{\psi_n^0\}$ is a complete set so

$$\psi_n^1 = \sum_{m \neq n} c_m^{(n)} \psi_m^0$$

$$\Downarrow$$

$$\sum_{m \neq n}\left(E_m^0 - E_n^0\right) c_m^{(n)} \psi_m^{(0)} = -\left(H^1 - E_n^1\right)\psi_n^0$$ (inner product with ψ_l^0)

$$\Downarrow$$

$$\sum_{m \neq n}\left(E_m^0 - E_n^0\right) c_m^{(n)} \langle \psi_l^0 | \psi_m^0 \rangle = -\langle \psi_l^0 | H^1 | \psi_n^0 \rangle + E_n^1 \langle \psi_l^0 | \psi_n^0 \rangle$$

Just look at $l \neq n$ ($l = n \rightarrow$ 1st-order pert. theory for the energy)

$$c_m^{(n)} = \frac{\langle \psi_m^0 | H^1 | \psi_n^0 \rangle}{E_n^0 - E_m^0}$$

$$\Downarrow$$

$$\psi_n^1 = \sum_{m \neq n} \frac{\langle \psi_m^0 | H^1 | \psi_n^0 \rangle}{\left(E_n^0 - E_m^0\right)} \psi_m^0$$