Lecture 11 - More Perturbation Theory

Have system $H = H^0 + \lambda H'$
H' = perturbation , λ = expansion parameter

$$\psi_n = \psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots$$

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2$$

Where $H \psi_n^0 = E_n^0 \psi_n^0$ unperturbed states
→ use as basis

Last time, derived
$$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle$$

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

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

Argued then E_n^1 makes some intuitive sense

$c_m^{(n)}$ formula more complicated:

See that (for small H') ψ_n is mostly ψ_n^0
"Mix in" some amount of other states

Amount of mixing is larger for states nearby in energy, smaller for states farther away

If you can estimate magnitude of $\langle H' \rangle$, can estimate how many states will be coupled

Note that if $E_n^0 = E_m^0$ for some m, we have trouble (unless $\langle \psi_m^0 | H' | \psi_n^0 \rangle = 0$)

Come back to that later.

For now, continue expansion, work out 2^{nd} order correction to energy E_n^2

Recall expansion

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

Second order terms:

I need parentheses!

$$H^0 \psi_n^{(2)} + H' \psi_n^{(1)} = E_n^{(2)} \psi_n^{(0)} + E_n^{(1)} \psi_n^{(1)} + E_n^{(0)} \psi_n^{(2)}$$

Take inner product with $\psi_n^{(0)}$:

$$E_n^{(0)} \langle \psi_n^{(0)} | \psi_n^{(2)} \rangle + \langle \psi_n^{(0)} | H' | \psi_n^{(1)} \rangle = E_n^{(2)} + E_n^{(1)} \langle \psi_n^{(0)} | \psi_n^{(1)} \rangle + E_n^{(0)} \langle \psi_n^{(0)} | \psi_n^{(2)} \rangle$$

So

$$E_n^{(2)} = \langle \psi_n^{(0)} | H' | \psi_n^{(1)} \rangle - E_n^{(1)} \langle \psi_n^{(0)} | \psi_n^{(1)} \rangle$$

But $\psi_n^{(1)} = \sum_{m \neq n} c_n^{(m)} \psi_n^{(1)}$

So $\langle \psi_n^{(0)} | \psi_n^{(1)} \rangle = 0$

$$E_n^{(2)} = \sum_{m \neq n} c_n^{(m)} \langle \psi_n^{(0)} | H' | \psi_m^{(0)} \rangle$$

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

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

Interpretation that doesn't work:

Perturbation gives amp: $\frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0}$ to be in state m.

$$\text{Prob} = \frac{|\langle \psi_m^0 | H' | \psi_n^0 \rangle|^2}{(E_n^0 - E_m^0)^2}$$

If it is in state m, get energy shift $\Delta E = E_m^{(0)} - E_n^{(0)}$

$$\text{Expect shift} = \text{Prob} \times \Delta E = - \frac{|\langle \psi_m^0 | H' | \psi_n^0 \rangle|^2}{E_n^0 - E_m^0}$$

Wrong sign!

Note if ψ_n^0 = ground state, then $E_m^0 > E_n^0$ for all m

so $E_n^{(2)}$ is always negative.

No one ever said QM has to make sense!

Right picture: when you couple two states, you always increase their energy splitting.

Upper state shifts up, lower state shifts down.

This is interesting and useful point, detour a bit to think about it.

Two Level System

Consider a system with just two quantum states
→ Maybe two states fairly close together, others all far away in energy, thus not coupled.

For just two states, we don't need perturbation theory, can solve exactly.

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Set up: $H = H^0 + H'$

Use basis states ψ_a^0, ψ_b^0

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

Convenient to write as a vector: $\psi = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$

Then $H^0 \psi = \alpha E_a^0 \psi_a^0 + \beta E_b^0 \psi_b^0$

Write as matrix $H^0 = \begin{bmatrix} E_a^0 & 0 \\ 0 & E_b^0 \end{bmatrix}$

What about H'?

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

So $\langle \psi_a^0 | H' | \psi \rangle = \alpha \langle \psi_a^0 | H' | \psi_a^0 \rangle + \beta \langle \psi_a^0 | H' | \psi_b^0 \rangle$

and $\langle \psi_b^0 | H' | \psi \rangle = \underbrace{\alpha \langle \psi_b^0 | H' | \psi_a^0 \rangle + \beta \langle \psi_b^0 | H' | \psi_b^0 \rangle}_{= \text{ Integrals we can evaluate}}$

Define $V_{aa} = \langle \psi_a^0 | H' | \psi_a^0 \rangle \quad V_{ab} = \langle \psi_a^0 | H' | \psi_b^0 \rangle$

$V_{bb} = \langle \psi_b^0 | H' | \psi_b^0 \rangle \quad V_{ba} = \langle \psi_b^0 | H' | \psi_a^0 \rangle = V_{ab}^*$