Lecture 12

Two-level system: to understand perturbation theory

Say just two states. Basis ψ_a^0, ψ_b^0

Hamiltonian $H = H^0 + H'$

$$H^0 \psi_a^0 = E_a^0 \psi_a^0$$
$$H^0 \psi_b^0 = E_b^0 \psi_b^0$$

Write general state $\psi = \alpha \psi_a^0 + \beta \psi_b^0$

Convenient to write as vector $\begin{bmatrix} \alpha \\ \beta \end{bmatrix}$

Can write H^0 as matrix:

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

or $$H^0 = \begin{bmatrix} E_a^0 & 0 \\ 0 & E_b^0 \end{bmatrix}$$

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

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

Then can write H' as matrix $\begin{bmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{bmatrix}$

Schro Eqn. $H\psi = E\psi$ becomes

$$\begin{bmatrix} E_a^0 + W_{aa} & W_{ab} \\ W_{ba} & E_b^0 + W_{bb} \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = E \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

Want to find eigenvalues E

Write $$\begin{bmatrix} \overbrace{E_a^0 + W_{aa}}^{A} - E & W_{ab} \\ W_{ba} & \underbrace{E_b^0 + W_{bb}}_{B} - E \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = 0$$

Determinant of matrix $= 0$

$$(A - E)(B - E) - |W_{ab}|^2 = 0$$

$$E^2 - E(A + B) + AB - |W_{ab}|^2 = 0$$

Quadratic:

$$E = \frac{1}{2}\left[A + B \pm \sqrt{(A+B)^2 - 4AB + 4|W_{ab}|^2} \right]$$

$$\boxed{E = \frac{1}{2}\left[A + B \pm \sqrt{(A-B)^2 + 4|W_{ab}|^2} \right]}$$

If $|W_{ab}| \ll |A-B|$, expand square root

$$E = \frac{1}{2}\left[A+B \pm (A-B)\left(1 + 2\frac{|W_{ab}|^2}{(A-B)^2}\right)\right]$$

$$E_+ = A + \frac{|W_{ab}|^2}{A-B}$$

$$E_- = B - \frac{|W_{ab}|^2}{A-B}$$

or

$$E_a = E_a^0 + W_{aa} + \frac{|W_{ab}|^2}{E_a^0 - E_b^0}$$

$$E_b = E_b^0 + W_{bb} + \frac{|W_{ab}|^2}{E_b^0 - E_a^0}$$

drop W's to this order

See this agrees with our perturbation theory results

$$E_a^1 = \langle \psi_a^0 | H' | \psi_a^0 \rangle = W_{aa}$$

$$E_a^2 = \frac{\langle \psi_a^0 | H' | \psi_b^0 \rangle \langle \psi_b^0 | H' | \psi_a^0 \rangle}{E_a^0 - E_b^0} = \frac{|W_{ab}|^2}{E_a^0 - E_b^0}$$

Funny behavior where 2nd-order term pushes energies apart:
because off-diagonal term in a matrix
pushes eigenvalues apart - not quite as mysterious

We use perturbation theory just because its hard
to diagonalize a matrix bigger than 2x2

Now, what happens if $E_a^0 = E_b^0 \equiv E^0$?

Then $\boxed{E = \frac{1}{2}\left[2E^0 + W_{aa} + W_{bb} \pm \sqrt{(W_{aa}-W_{bb})^2 + 4|W_{ab}|^2}\right]}$

$$= E^0 + E^1$$

First order correction

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

can't simplify in general

However, if $W_{ab} = 0$, then $E' = W_{aa}$ or W_{bb}
same as normal nondegenerate result

→ Good to pick ψ_a^0 and ψ_b^0 so that
$W_{ab} = 0$

Since $E_a^0 = E_b^0$, can use any linear combination
of states for basis.

Trick: find some other operator Q that commutes
with H^0 and H'
(Parity, angular momentum, linear momentum
are good things to try)

Then use eigenstates of Q as basis:
since $[Q, H'] = 0$, guaranteed that $W_{ab} = 0$

If you can't find such an operator Q, just
use general formula

Note, sometimes have $0 < |E_a^0 - E_b^0| \sim W_{ab}$

Then must use general formula for E.
Really, perturbation theory doesn't apply