Lecture 12

Two-level system: to understand perturbation theory

Say just two states: Basis $|a\rangle$, $|b\rangle$

Hamiltonian $H = H^0 + H'$

$H^0 |a\rangle = E_a |a\rangle$
$H^0 |b\rangle = E_b |b\rangle$

Write general state $|\psi\rangle = \alpha |a\rangle + \beta |b\rangle$

Convenient to write as vector

$\begin{bmatrix} \alpha \\ \beta \end{bmatrix}$

Can write $H^0$ as matrix:

$|\psi\rangle = \alpha |a\rangle + \beta |b\rangle$

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

What about $H'$?

$H' |a\rangle = \alpha H' |a\rangle + \beta H' |b\rangle$

So $\langle a | H' |a\rangle = \alpha \langle a | H' |a\rangle + \beta \langle a | H' |b\rangle$

and $\langle b | H' |b\rangle = \alpha \langle b | H' |b\rangle + \beta \langle b | H' |b\rangle$

Integrals we can evaluate
Define $W_{aa} = \langle 2\alpha | H | 2\alpha \rangle$ $W_{ab} = \langle 2\alpha | H | 12\beta \rangle$

$W_{ba} = <2\beta | H | 12\alpha \rangle$ $W_{bb} = <2\beta | H | 12\beta \rangle$

Then we can write $H'$ as matrix

$$\begin{bmatrix}
W_{aa} & W_{ab} \\
W_{ba} & W_{bb}
\end{bmatrix}$$

Schrödinger Eqn. $H' + E2 = E$ becomes

$$\begin{bmatrix}
E_0 + W_{aa} & W_{ab} \\
W_{ba} & E_0 + W_{bb}
\end{bmatrix} \begin{bmatrix}
\alpha \\
\beta
\end{bmatrix} = E \begin{bmatrix}
\alpha \\
\beta
\end{bmatrix}$$

Want to find eigenvalues $E$

Write

$$\begin{bmatrix}
E_0 + W_{aa} - E & W_{ab} \\
W_{ba} & E_0 + W_{bb} - E
\end{bmatrix} \begin{bmatrix}
\alpha \\
\beta
\end{bmatrix} = 0$$

Determinate of matrix $= 0$

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

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

Quadratic:

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

$$E = \frac{1}{2} \left[ A + B \pm \sqrt{(A - B)^2 + 4|W_{ab}|^2} \right]$$
If \(|W_{a3}| < c |A-B|\), expand square root

\[
E = \frac{1}{2} \left[ A+B \pm \sqrt{(A-B)\left(1 + 2 \frac{|W_{a3}|}{|A-B|^2}\right)} \right]
\]

\[
E_+ = A + \frac{|W_{a3}|}{A-B}
\]

\[
E_- = B - \frac{|W_{a3}|}{A-B}
\]

or

\[
E_a = E_0^a + W_{aa} + \frac{|W_{a3}|}{E_0 - E_0^a}
\]

\[
E_b = E_0^b + W_{bb} + \frac{|W_{a3}|}{E_0 - E_0^b}
\]

Drop W's to this order.

See this agrees with our perturbation theory results:

\[
E_a' = \langle \phi_0^a | H' | \phi_0^a \rangle = W_{aa}
\]

\[
E_a'' = \frac{\langle \phi_0^a | H'' | \phi_0^a \rangle}{E_0 - E_0^a} = \frac{|W_{a3}|^2}{E_0 - E_0^a}
\]

Fancy 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 it's hard

to diagonalize a matrix bigger than 2x2

Now, what happens if \(E_0^a = E_0^b = E_0\)?

Then

\[
E = \frac{1}{2} \left[ 2E_0 + W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{a3}|^2} \right]
\]

\[
= E_0 + E_1
\]
First order correction

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

can't simplify in general

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

\( \Rightarrow \) Good to pick \( 2\theta_0 \) and \( 2\alpha_0 \) 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 \( \Pi \) that commutes
with \( H^0 \) and \( H' \)

(Parity, angular momentum, linear momentum
are good things to try)

Then use eigenstates of \( \Pi \) as basis:

since \( [\Pi, H'] = 0 \) guaranteed that \( W_{ab} = 0 \)

If you can't find such an operator \( \Pi \), just
use general formula

Note, sometimes have \( 0 < |E_a^0 - E_b^0| < \infty \) \( W_{ab} \)

Then must use general formula for \( E \),
really, perturbation theory doesn't apply