Lecture II

Last time, started perturbation theory by discussing **two-level system**

Two levels \( |1\rangle, |2\rangle \)

arbitrary Hamiltonian

\[
\begin{bmatrix}
H_{11} & H_{12} \\
H_{21} & H_{22}
\end{bmatrix}
\]

found general solution for eigenenergies

\[
E_\pm = \frac{1}{2} \left[ H_{11} + H_{22} \pm \sqrt{\Delta^2 + V^2} \right]
\]

\[\Delta = H_{22} - H_{11}\]
\[V = 2|H_{12}|\]

and eigenvalues eigenstates

\[|\varphi_\pm\rangle = C_{\pm 1} |1\rangle + C_{\pm 2} |2\rangle\]

\[C_{\pm 1} = \frac{1}{\sqrt{2}} \left( 1 \pm \frac{\Delta}{\sqrt{\Delta^2 + V^2}} \right)^{1/2}\]

\[C_{\pm 2} = \frac{i}{\sqrt{2}} \left( 1 \pm \frac{\Delta}{\sqrt{\Delta^2 + V^2}} \right)^{1/2} e^{-i\phi}\]

for \( e^{i\phi} = \frac{H_{12}}{|H_{12}|} \)

Note, these solutions are exact

Let's look at how they behave in perturbation limit
Suppose \( H = H^{(0)} + H' \)

\[
H^{(0)} = \begin{bmatrix}
E_1^{(0)} & 0 \\
0 & E_2^{(0)}
\end{bmatrix}
\]

already diagonal in original basis

\[
H' = \begin{bmatrix}
H_{11}' & H_{12}' \\
H_{21}' & H_{22}'
\end{bmatrix}
\]

"small"

Then take our solutions, and Taylor expand for small \( H' \)

Energies: \( E_\pm = \frac{1}{2} \left[ E_1^{(0)} + E_2^{(0)} + H_{11}' + H_{22}' \pm \sqrt{\left[ E_2^{(0)} + H_{22}' - E_1^{(0)} - H_{11}' \right]^2 + 4 |H_{12}'|^2} \right] \)

Want to expand \( \sqrt{\frac{1}{\Delta + \Delta'} \right) \): rewrite as

\[
\frac{1}{\sqrt{(\Delta + \Delta')^2 + V'^2}}
\]

\[
\Delta = \frac{E_2^{(0)} - E_1^{(0)}}{2}
\]

\[
\Delta' = H_{22}' - H_{11}'
\]

\[
V' = 2 |H_{12}'|
\]

\[
= \left( \Delta^2 + 2 \Delta \Delta' + \Delta'^2 + V'^2 \right)^{1/2}
\]

Run into a problem:

\( E_1^{(0)} \) and \( E_2^{(0)} \) might be large, but \( E_2^{(0)} - E_1^{(0)} \) could = 0

Can't Taylor expand if \( H' \) isn't small compared to \( \Delta \)
Have to consider different cases:

First, say $|\Delta| > 10^{-1}, V$

Then use expansion $\sqrt{1+x} \approx 1 + \frac{x}{2} + O(x^2)$

So \[ \sqrt{\Delta^2 + 2 \Delta \Delta' + \Delta'^2 + V^2} \approx |\Delta| \left(1 + \frac{2 \Delta'}{\Delta} \right)^{1/2} \]

\[ \approx |\Delta| + \frac{|\Delta|}{\Delta} \Delta' \]

Let's take $\Delta > 0$ (switch state labels if not)

then \[ \sqrt{\Delta} \rightarrow \Delta + \Delta' \]

and

\[ E_\pm \rightarrow \frac{1}{2} \left[ E_1^{(0)} + E_2^{(0)} + H_{11}' + H_{22}' \pm \left( E_2^{(0)} - E_1^{(0)} + H_{22}' - H_{11}' \right)^2 \right] \]

\[ E_+ = E_2^{(0)} + H_{22}' \]

\[ E_- = E_1^{(0)} + H_{11}' \]

See that energy of state $1\delta$ is shifted by $\langle n | H' | n \rangle$

Pretty intuitive

Note $H_{12}'$ has no effect (to 1st order)

What about 2nd order?

Can do same 1st order expansion for eigenstates

you get to work through in HW!

This is why I introduced two-level system:

So we could see a concrete example of how Taylor expansion works.

Now want to generalize to arbitrary system...
Consider general system with \( H = H^{(0)} + \lambda H' \)

actually write \( = H^{(0)} + \lambda H' \) \( H^{(0)} \) diagonal

\( \lambda = 1 \), "dummy parameter"

makes it easier to count powers of \( H' \)

Expect eigenstates to have form

\[
\psi_n = \psi^{(0)}_n + \lambda \psi^{(1)}_n + \lambda^2 \psi^{(2)}_n + \ldots
\]

\[
E_n = E^{(0)}_n + \lambda E^{(1)}_n + \lambda^2 E^{(2)}_n + \ldots
\]

where \( \psi^{(0)}_n \) = eigenstate of \( H^{(0)} \) with energy \( E^{(0)}_n \)

Develop procedure to get higher order terms

Have \( H \psi_n = E_n \psi_n \)

\[
(H^{(0)} + \lambda H') (\psi^{(0)}_n + \lambda \psi^{(1)}_n + \lambda^2 \psi^{(2)}_n + \ldots)
\]

\[
= (E^{(0)}_n + \lambda E^{(1)}_n + \lambda^2 E^{(2)}_n + \ldots) (\psi^{(0)}_n + \lambda \psi^{(1)}_n + \lambda^2 \psi^{(2)}_n + \ldots)
\]

Collect like powers of \( \lambda \):

\[
H^{(0)} \psi^{(0)}_n + \lambda \left[ H^{(0)} \psi^{(1)}_n + H^{(0)} \psi^{(2)}_n + \ldots \right] + \lambda^2 \left[ H^{(0)} \psi^{(2)}_n + H^{(0)} \psi^{(3)}_n + \ldots \right] + \ldots
\]

\[
= E^{(0)}_n \psi^{(0)}_n + \lambda \left[ E^{(1)}_n \psi^{(1)}_n + E^{(1)}_n \psi^{(2)}_n + \ldots \right] + \lambda^2 \left[ E^{(2)}_n \psi^{(2)}_n + E^{(2)}_n \psi^{(3)}_n + \ldots \right] + \ldots
\]
\( \lambda^0 \) terms:
\[ H_n^{(0)} \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)} \]
\( \checkmark \)

\( \lambda^1 \) terms:
\[ H' \psi_n^{(0)} + H^{(0)} \psi_n^{(1)} = E_n^{(1)} \psi_n^{(0)} + E_n^{(0)} \psi_n^{(1)} \]

* Solve this for \( E_n^{(1)} \) and \( \psi_n^{(1)} \).

* Multiply by \( \psi_n^{(0)} \) and integrate

\[
\langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle + \langle \psi_n^{(0)} | H^{(0)} | \psi_n^{(1)} \rangle
\]

\[ = E_n^{(1)} \langle \psi_n^{(0)} | \psi_n^{(0)} \rangle + E_n^{(0)} \langle \psi_n^{(0)} | \psi_n^{(1)} \rangle \]

* Use \( \langle \psi_n^{(0)} | H^{(0)} = \langle \psi_n^{(0)} | E_n^{(0)} \rangle \)

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

So
\[
\langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle + E_n^{(0)} \langle \psi_n^{(0)} | \psi_n^{(1)} \rangle
\]

\[ = E_n^{(1)} + E_n^{(0)} \langle \psi_n^{(0)} | \psi_n^{(1)} \rangle \]

Or
\[ E_n^{(1)} = \langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle \]

Same as result for two-level system:

First-order correction to energy of state \( n \)

is expectation value of perturbation in

that state.

Simple but quite powerful.
Let's get correction to state, \( \psi _{n}^{(1)} \):

Rewrite \( \psi \) as

\[
[ H_{n}^{(0)} - E_{n}^{(0)} ] \psi _{n}^{(1)} = - [ H' - E_{n}^{(1)} ] \psi _{n}^{(0)}
\]

Expand \( \psi _{n}^{(1)} \) in terms of \( \psi _{n}^{(0)} \) basis:

\[
\psi _{n}^{(1)} = \sum _{m \neq n} C_{nm} \psi _{m}^{(0)}
\]

a) Leave out \( m=n \) term, since we are looking for correction to \( \psi _{n}^{(0)} \). 

\( C_{nn} \) term is really part of zero order solution.

b) My notation different from book: 

Griffiths has \( C_{nm} = C_{m}^{(n)} \) confusing.

Plus expansion into eqn:

\[
\sum _{m \neq n} C_{nm} ( E_{m}^{(0)} - E_{n}^{(0)} ) \psi _{m}^{(0)} = - ( H' - E_{n}^{(1)} ) \psi _{n}^{(0)}
\]

Take inner product with \( \psi _{l}^{(0)} \):

\[
\sum _{m \neq n} C_{nm} ( E_{m}^{(0)} - E_{n}^{(0)} ) \langle \psi _{l}^{(0)} | \psi _{m}^{(0)} \rangle = - \langle \psi _{l}^{(0)} | H' | \psi _{n}^{(0)} \rangle \\
+ E_{n}^{(1)} \langle \psi _{l}^{(0)} | \psi _{n}^{(0)} \rangle
\]

Use \( \langle \psi _{l}^{(0)} | \psi _{m}^{(0)} \rangle = \delta _{lm} \)

\[
C_{ml} ( E_{l}^{(0)} - E_{n}^{(0)} ) = - \langle \psi _{l}^{(0)} | H' | \psi _{n}^{(0)} \rangle + E_{n}^{(1)} \langle \psi _{l}^{(0)} | \psi _{n}^{(0)} \rangle
\]

If \( n=l \), back to \( E_{n}^{(1)} = \langle \psi _{n}^{(0)} | H' | \psi _{n}^{(0)} \rangle \) as before.