Degenerate Pert'n Theory

Now let's tackle the degenerate case.

$$H^{(0)} = \begin{pmatrix} \ddots & 0 & 0 \\ 0 & \begin{matrix} E_n^{(0)} & & 0 \\ & E_n^{(0)} & \\ 0 & & \ddots \; E_n^{(0)} \end{matrix} & 0 \\ 0 & \underbrace{0}_{D \; (N \times N)} & \ddots \end{pmatrix} + \varepsilon V \qquad E_{m_1}^{(0)} = E_{m_2}^{(0)}, \quad m_1, m_2 \in D$$

Our previous treatment breaks down b/c we assumed $E_m^{(0)} \neq E_n^{(0)} \;\; \forall m,n$

Formulas break down

$$\begin{cases} |n^{(1)}\rangle = \sum_{m \neq n} \frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}} |m^{(0)}\rangle \\ E_n^{(2)} = \sum \frac{|V_{mn}|^2}{E_n^{(0)} - E_m^{(0)}} \end{cases}$$

division by 0!

Also $E_n^{(1)} = \langle n^{(0)} | V | n^{(0)} \rangle$

is ambiguous $\rightarrow$ which $|n^{(0)}\rangle$ do we use??

w/ degen $H^{(0)}$, have eigen bases under unitary transf.

$$D \rightarrow U \cdot D$$

$$\begin{pmatrix} |n_1\rangle \\ \vdots \\ |n_D\rangle \end{pmatrix} \rightarrow U \begin{pmatrix} |n_1\rangle \\ \vdots \\ |n_D\rangle \end{pmatrix}.$$

Where did we go wrong in general derivn?

$$\left(H^{(0)}+\varepsilon V\right)|n\rangle = \left(E_n^{(0)}+\varepsilon\Delta_n\right)|n\rangle$$

$\langle n^{(0)}| \times (\cdots = \cdots) \implies \boxed{\Delta_n = \langle n^{(0)}|V|n\rangle}$ OK

$m\neq n \quad \langle m^{(0)}| \times (\cdots = \cdots) \implies E_m^{(0)}\langle m^{(0)}|n\rangle + \varepsilon \langle m^{(0)}|V|n\rangle$

$$= E_n^{(0)}\langle m^{(0)}|n\rangle + \varepsilon\Delta_n\langle m^{(0)}|n\rangle$$

$$\boxed{c_{nm} = \frac{\varepsilon\left(V_{mn} + \sum_{m'\neq n} c_{nm'}V_{mm'}\right)}{E_n^{(0)} - E_m^{(0)} + \varepsilon\Delta_n}} \quad (*) \qquad \boxed{\langle m^{(0)}|n\rangle = \frac{\varepsilon\langle m^{(0)}|V|n\rangle}{E_n^{(0)} - E_m^{(0)} + \varepsilon\Delta_n}}$$

concise master eqn for all m!

Before we took $E_m^{(0)} - E_n^{(0)}$ as $O(1)$ & expanded in ε,

$$\langle m^{(0)}|n\rangle = \frac{\varepsilon\langle m^{(0)}|V|n^{(0)}\rangle}{E_m^{(0)} - E_n^{(0)}} + \cdots$$

Now if $E_m^{(0)} = E_n^{(0)}$ it fails!

instead get

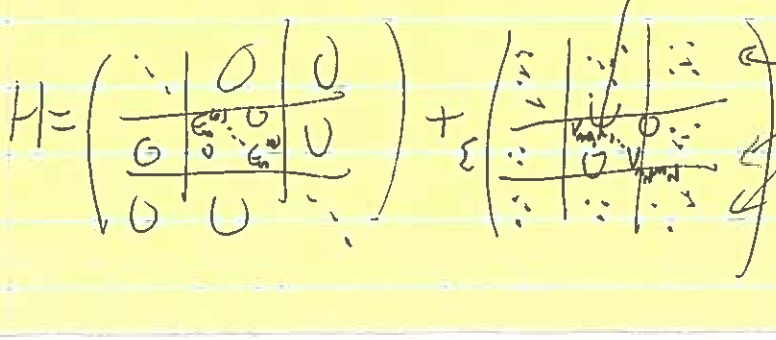
$$\boxed{\langle n^{(0)}|n\rangle = 0\langle m^{(0)}|V|n\rangle} \quad \begin{matrix} m\neq n \\ m\in D \end{matrix}$$

At 0th order $\implies$

$$\langle n^{(0)}|\left(\cancel{|n^{(0)}\rangle} + \varepsilon|n^{(1)}\rangle + \cdots\right) = \langle m^{(0)}|V|n^{(0)}\rangle + \varepsilon\langle n^{(0)}|V|n^{(1)}\rangle + \cdots$$

$$\longrightarrow \boxed{\langle m^{(0)}|V|n^{(0)}\rangle = 0}$$

correct basis is where V is diagonal in D!



off diag still non zero

then $E_n^{(1)} = \langle n^{(0)}|V|n^{(0)}\rangle$ is unambiguous!

~~Assume V pert'n splits energies @ 1st order.~~ ~~looks degen~~

- What about $\epsilon_n^{(2)}$?

(△) $\epsilon_n^{(2)} = \langle n^{(0)} | V | n^{(1)} \rangle$

$$= \sum_{m \notin D} \frac{|V_{mn}|^2}{\epsilon_n^{(0)} - \epsilon_m^{(0)}} \quad ✓.$$

$$|n^{(1)}\rangle = \sum_{m \notin D} \frac{V_{mn}}{\epsilon_n^{(0)} - \epsilon_m^{(0)}} |m^{(0)}\rangle + \sum_{\substack{m \in D \\ m \neq n}} c_{mn} |m^{(0)}\rangle$$

don't contribute since V_D is diag!

- What about $|n^{(1)}\rangle\Big|_D$?

$\longrightarrow$ c_{mn} for $m \in D$?

(⊛) $\Delta_n \langle m^{(0)} | n \rangle = \langle m^{(0)} | V | n \rangle$.

Need to unpack (⊛):

$$\Delta_n c_{mn} = \sum_{m' \notin D} \frac{V_{m'n} V_{mm'}}{\epsilon_n^{(0)} - \epsilon_{m'}^{(0)}} + \underbrace{V_{mm}}_{\epsilon_m^{(1)}} c_{mn}$$

$\Delta_n \to V_{nn} = \epsilon_n^{(1)}$

$$\Longrightarrow \boxed{c_{mn} = \sum_{m' \notin D} \frac{V_{m'n} V_{mm'}}{\left(\epsilon_n^{(0)} - \epsilon_{m'}^{(0)}\right)\left(\epsilon_n^{(1)} - \epsilon_m^{(1)}\right)}}$$

$\longleftarrow$ note: requires degen is lifted @ 1st order!!

- Comment: c_{mn} looks 2nd order (V^2) but $\epsilon_n^{(1)} - \epsilon_m^{(1)}$ in denom $\Rightarrow \frac{\epsilon^2}{\epsilon} = \epsilon$ 1st order!

Q: what if it's not?

HW: Check get same answer for $c_{mn}^{(1)}$ this way

- More generally, can absorb V_D into defn of $H^{(0)}$

$$H^{(0)} = \begin{pmatrix} \ddots & & \\ & \begin{matrix} \epsilon_n^{(0)} + \epsilon V_{11} & 0 \\ & \ddots \\ 0 & \epsilon_n^{(0)} + \epsilon V_{NN} \end{matrix} & \\ & & \ddots \end{pmatrix} \quad \epsilon \tilde{V} = \epsilon \begin{pmatrix} \xi & \xi & \xi \\ \xi & 0 & \xi \\ \xi & \xi & \xi \end{pmatrix}.$$

Then if degen lifted @ 1st order, can apply non-degen pert'n thy to this redefined system!

Summary

For degen pert'n thy

- Diagonalize V' on degen subspace
  These are the "good" basis vectors
- If lifted @ 1^{st} order, apply non degen pert'n thy to redefined system
- Be careful about orders in ε!
  - need 2^{nd} orders in ε to get 1^{st} order states!
- If not lifted @ 1^{st} order, ~~can't use formulas for~~ $\cancel{E_n^{(1)}}$ ~~&~~ $\cancel{E_n^{(2)}}$. need to work even harder to identify "good" basis...