WEEK 4: Degenerate TIPT

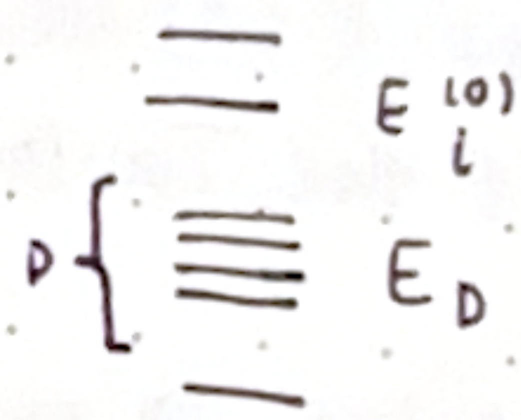
We previously assumed energy levels are well separated / non-degenerate. Say now instead that unperturbed eigenstates in set D <u>all</u> have energy E_D.

As before: $\hat{H} = \hat{H}_0 + \hat{V}$, $\hat{H}_0 |\varphi_i\rangle = E_i^{(0)} |\varphi_i\rangle$. If we use the same methods as before, we run into divide-by-0 errors.

Instead, define $\hat{P} = \sum_{i \in D} |\varphi_i\rangle\langle\varphi_i|$ and $\hat{Q} = \hat{1} - \hat{P}$. Then we can write:

$$\hat{V} = (\hat{P}+\hat{Q})\hat{V}(\hat{P}+\hat{Q}) = \hat{P}\hat{V}\hat{P} + \hat{P}\hat{V}\hat{Q} + \hat{Q}\hat{V}\hat{P} + \hat{Q}\hat{V}\hat{Q} \quad \text{or concisely,}$$

$$= \hat{V}_{PP} + \hat{V}_{PQ} + \hat{V}_{QP} + \hat{V}_{QQ}$$



The space of $\hat{Q}$ is "everything outside of D" and the space of $\hat{P}$ is formed by D, so $\hat{V}_{PP}$ takes an arbitrary vector, projects it into D, applies $\hat{V}$, projects it into D again.
Likewise, $\hat{V}_{PQ}$ applies $\hat{V}$ to a vector <u>outside</u> of D, then brings it into D, $\hat{V}_{QP}$ applies $\hat{V}$ to a vector in D and brings it out of D, and $\hat{V}_{QQ}$ applies $\hat{V}$ to a vector outside of D and keeps it outside of D.

<u>So</u> $\hat{V}_{PP}$ is the only part of the perturbation that operates <u>entirely</u> in D. Thus it is the only component that <u>could</u> break up degeneracy in the model Hamiltonian's degenerate space D.

$\hat{V}_{PQ}$ can only <u>introduce</u> more degeneracy into D, $\hat{V}_{QP}$ (I guess) can't be relied on to take <u>every</u> state in D out of D, and $\hat{V}_{QQ}$ does not involve D at all.

Thus we define a <u>new</u> model Hamiltonian $\hat{H}_0' = \hat{H}_0 + \hat{V}_{PP}$ and assume it now has <u>no</u> degeneracy in D.

<u>AN ASIDE ON MOTIVATING ISSUES:</u> We encounter divide-by-0 issues with degenerate states in our original approach to TIPT. We actually also see this issue when two energy levels are just <u>very close</u>: $|V_{ij}| \gtrsim |E_i - E_j|/2$.

Say we have a system with states $\{|1\rangle, |2\rangle\}$, and Hamiltonian:

$$\mathbb{H} = \begin{bmatrix} E_1 & V \\ V^* & E_2 \end{bmatrix}$$ where V is some interaction term. We want to diagonize $\mathbb{H}$.

We can alternatively say: $\mathbb{H} = E_1 \mathbb{1} + \begin{bmatrix} 0 & V \\ V^* & \Delta \end{bmatrix}$ where $\Delta \equiv E_2 - E_1$, to find the eigenvalues / eigenvectors of $\mathbb{H}$, we can just find the eigen-values/vectors for $\begin{bmatrix} 0 & V \\ V^* & \Delta \end{bmatrix}$ (tho add E_1 to the eigen values).

So: $\begin{vmatrix} -\varepsilon & V \\ V^* & \Delta - \varepsilon \end{vmatrix} = \varepsilon(\varepsilon - \Delta) - |V|^2 = 0$

$$\varepsilon^2 - \Delta\varepsilon - |V|^2 = 0$$

using quadratic formula: $\varepsilon_\pm = \frac{\Delta}{2} \pm \sqrt{\frac{\Delta^2}{4} + |V|^2}$

If $\Delta \neq 0$, $\varepsilon_\pm = \frac{\Delta}{2}\left\{1 \pm \sqrt{1 + \left|\frac{2V}{\Delta}\right|^2}\right\}$

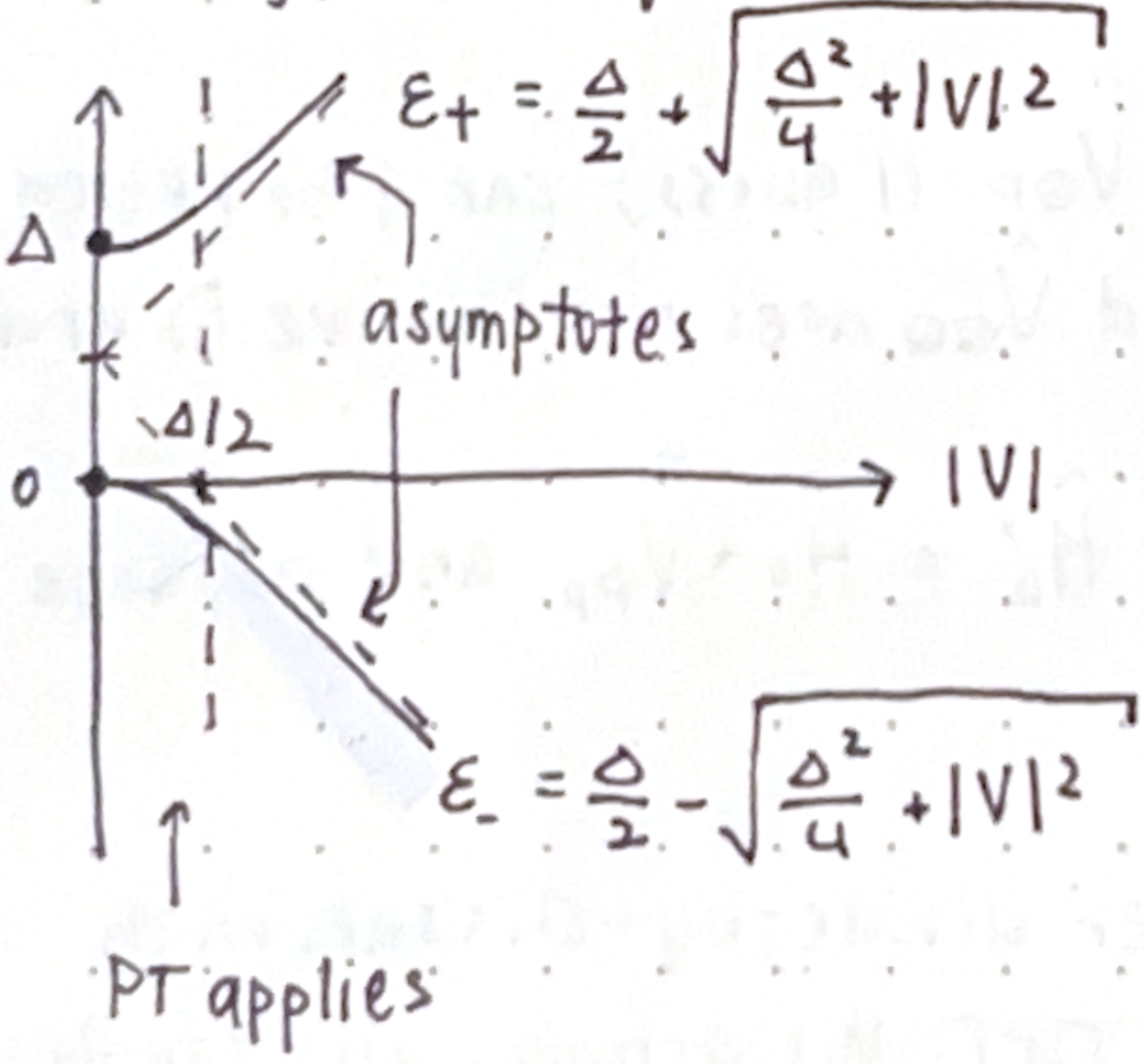
Recall that in our previous approach to TIPT, we want to write the true energies $E(\lambda)$ as expansions of powers of λ. We cannot do this, evidently, if the Taylor series does not converge for these energies!

Thus we want $\varepsilon_\pm$ to converge. However $\sqrt{1+x}$ has a radius of convergence. Each term in the taylor expansion comes closer and closer to approximating $\sqrt{1+x}$ ONLY for $x = -1$ to $x = 1$.

So, $\left|\frac{2V}{\Delta}\right|^2$ has to be between -1 and 1. Clearly it is always positive, so we just need to make sure it is less than 1:

$$\left|\frac{2V}{\Delta}\right|^2 < 1 \rightarrow 2|V| < \Delta \rightarrow |V| < \frac{\Delta}{2}$$

Plotting these eigenvalues as a function of $|V|$:



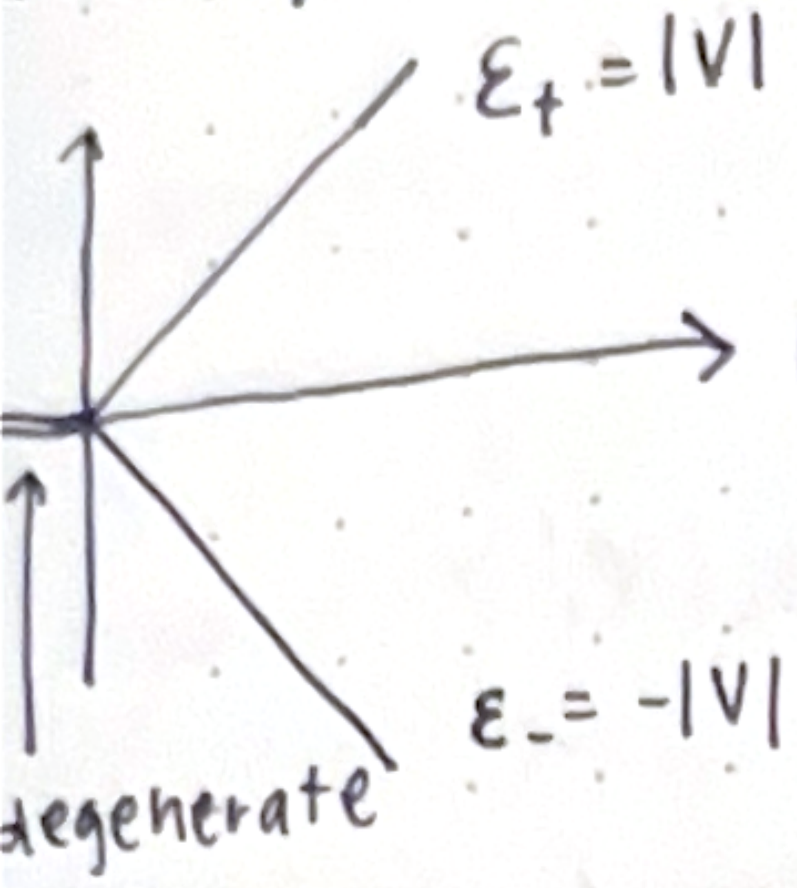
Note for $|V| \ll \Delta$: $\varepsilon_\pm \cong \frac{\Delta}{2}\left\{1 \pm 1 \pm \left(\frac{2|V|}{\Delta}\right)^2\right\}$ or that for $|V| \ll \Delta$,
$\varepsilon_+ \cong \Delta + 2|V|^2/\Delta$ and $\varepsilon_- \cong -2|V|^2/\Delta$

Hence we see quadratic behavior near the origin.

For $|V| \gg \Delta$, however, $\varepsilon_\pm \cong \frac{\Delta}{2}\left\{1 \pm \frac{2|V|}{\Delta}\overbrace{\left(1 + \frac{1}{8}\frac{\Delta^2}{|V|^2}\right)}^{\text{very small correction}}\right\}$

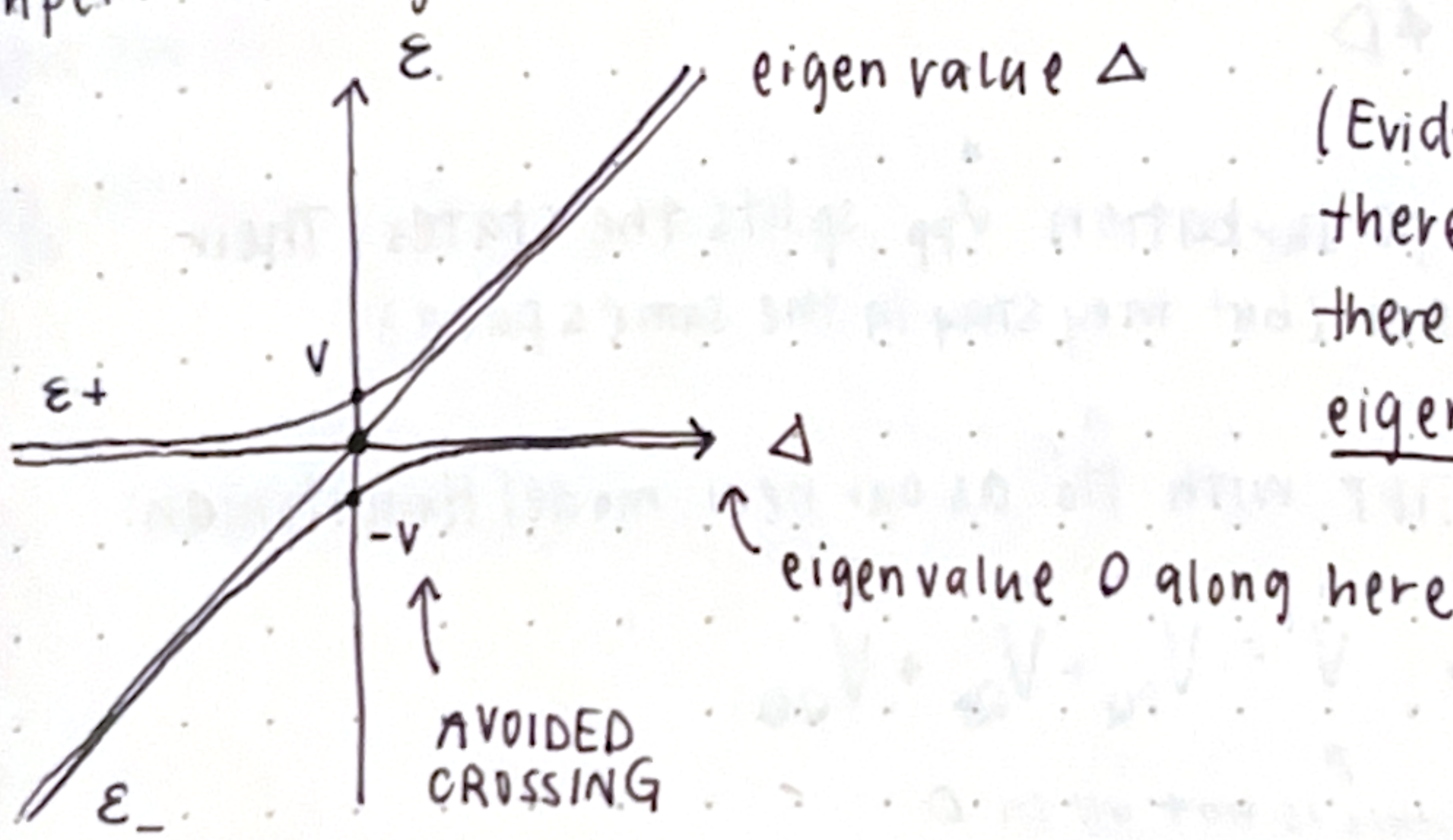
and so we see linear behavior to the right of $\Delta/2$. This linear separation is a hallmark of degenerate <u>or</u> strongly interacting states.

For degenerate states where $\Delta = 0$, $\varepsilon_\pm = \pm|V|$, so we have:



What if we keep the interaction/perturbation V fixed, but change the value of $\Delta = E_2 - E_1$? In this case, the eigenfunctions/eigenvalues slide up and down.

Without perturbation, the matrix is $\begin{bmatrix} 0 & 0 \\ 0 & \Delta \end{bmatrix}$, since $V = 0$. Thus unperturbed eigenvalues are 0 and Δ. We already know $\varepsilon_\pm$ wrt Δ also



(Evidently with perturbation, there is no crossing, so there are no <u>degenerate eigenvalues!</u>)

If $|\Delta| >> |V|$, $\varepsilon_\pm \approx \frac{\Delta}{2} \pm \frac{|\Delta|}{2}\sqrt{1 + \frac{4V^2}{\Delta^2}} \approx 0$ or Δ. When Δ is negative, $\varepsilon_- \approx \Delta$ and $\varepsilon_+ \approx 0$.

very small

When Δ is positive, $\varepsilon_+ \approx \Delta$ and $\varepsilon_- = 0$.

Essentially, the perturbed eigenstates begin by following some unperturbed values, then at the crossing they (kind of) swap:

$$\hat{H}|\pm\rangle = \varepsilon_\pm|\pm\rangle, \quad |\pm\rangle = a_\pm|1\rangle + b_\pm|2\rangle, \quad |a_\pm|^2 + |b_\pm|^2 = 1$$

$$|+\rangle : |1\rangle \rightarrow |2\rangle \quad \text{and} \quad |-\rangle : |2\rangle \rightarrow -|1\rangle$$

$|+\rangle$ and $|-\rangle$ "change character".

BACK TO DEGENERATE TIPT

same as $\hat{H}_0$

$\forall i \in D,\ \hat{H}_0' |\varphi_i'\rangle = E_i |\varphi_i'\rangle$ and $\forall j \notin D,\ \hat{H}_0' |\varphi_j\rangle = E_j^{(0)} |\varphi_j\rangle$

$\hat{H}_0' = \hat{H}_0 + \lambda \hat{V}_{PP}$ $\quad \hat{H}_0' |\varphi_i'\rangle$ is:

$$(\hat{H}_0 + \lambda \hat{V}_{PP}) |\varphi_i'\rangle = (E_D + \lambda V_i) |\varphi_i'\rangle$$

Here we assume we have diagonal $\hat{V}_{PP}$ so $\hat{V}_{PP} |\varphi_i'\rangle = v_i |\varphi_i'\rangle$ ($|\varphi_i'\rangle$ are the eigenstates of $\hat{V}_{PP}$ in D).

perturbation induces linear splitting!

Thus $E_i' = E_D + \lambda V_i$

We already defined $\hat{Q}$, we now define $\hat{Q}_i' = \hat{1} - |\varphi_i'\rangle\langle\varphi_i'|$ or the projector that excludes $|\varphi_i'\rangle$ only. This is equal to:

$$\sum_{\substack{j \in D \\ j \neq i}} |\varphi_j'\rangle\langle\varphi_j'| + \sum_{j \notin D} |\varphi_j\rangle\langle\varphi_j|$$

Again, we hope the extra perturbation $\hat{V}_{PP}$ splits the states. Their energies should be different (but they stay in the same space).

We can use normal ass TIPT with $\hat{H}_0'$ as our new model Hamiltonian:

$$E_i'^{(1)} = \langle\varphi_i'| \hat{V}' |\varphi_i'\rangle, \quad \hat{V}' = \hat{V}_{PQ} + \hat{V}_{QP} + \hat{V}_{QQ}$$

these are in D $\qquad$ this is not all in D

$= 0$

so the corrected energy to first order is $E_i' = E_D + \lambda V_i$

The corresponding $|\psi_i'^{(1)}\rangle$ is:

$$\underbrace{\sum_{\substack{j \in D \\ j \neq i}} |\varphi_j'\rangle \frac{\langle\varphi_j'| \hat{V}' |\varphi_i'\rangle}{E_i' - E_j'}}_{\substack{=0 \text{ again because} \\ \hat{V} \text{ is not all in D}}} + \sum_{j \notin D} |\varphi_j\rangle \frac{\langle\varphi_j| \hat{V} |\varphi_i\rangle}{E_i' - E_j^{(0)}}$$

And the second order energy correction is:

$$E_i^{'(2)} = \sum_{j \notin D} \frac{\langle \varphi_i' | \hat{V} | \varphi_j \rangle \langle \varphi_j | \hat{V} | \varphi_i' \rangle}{E_i' - E_j^{(0)}}$$

if we want to use $\lambda \hat{V}$ instead, $E_i^{'(2)}$ has a λ^2 coefficient and

$E_i^{'(0)} = E\lambda^0 + V_i \lambda^1$ and now $E_i^{'(2)}$ has λ^2, so we get a neat expansion in terms of λ^n.

Of course, remember this rides on the assumption that $\hat{V}_{PP}$ breaks up the degeneracy in $\hat{H}_0$, so <u>NONE of the V_i may coincide</u>.

Notice that $\hat{H}_0'$ depends on λ. Thus $|\Psi_i'^{(1)}\rangle$ scales in λ and:

- We may miss contributions to $|\Psi\rangle$ that are linear in λ
- These missing terms can come from <u>inside</u> D.

Let's see this:

$$|\Psi_i'^{(2)}\rangle = (\hat{G}_{Q_i'}(E_i')\hat{V}')^2|\varphi_i'\rangle - \underbrace{E_i'^{(2)}}_{=0}\hat{G}^2_{Q_i'}(E_i')\hat{V}'|\varphi_i'\rangle$$

$$= \left(\frac{1}{E_i' - \hat{H}_0'}\hat{Q}_i'\hat{V}'\right)^2|\varphi_i'\rangle$$