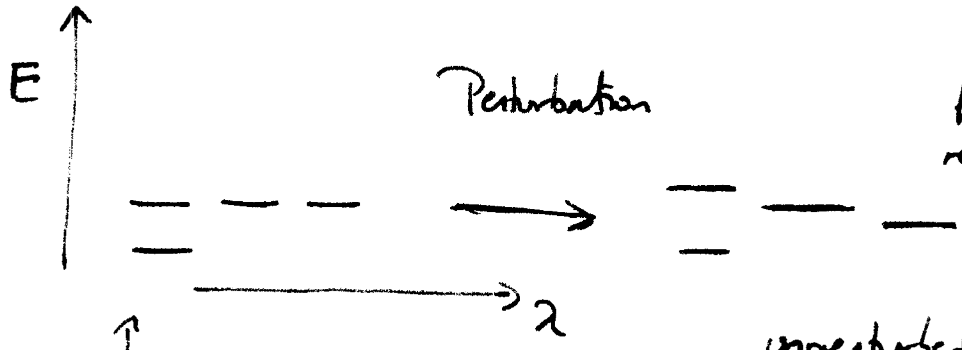
Degenerate Perturbation Theory.



How do these perturbed states reduce to the unperturbed ones as $\lambda \to 0$? In other words, what linear combination of the unperturbed states is the $\lambda \to 0$ limit of the perturbed ones.

eigenstates of H_0 and some other observable A.

$|k^{(0)}\rangle \leftarrow$ collective index.

Note also that if we try to blindly apply our previous results to the degenerate subspace of states we run into problems with energy denominators:

$$\frac{V_{nk}}{E_n^{(0)} - E_k^{(0)}}$$ is singular when n, k are in the degenerate subspace.

We will find that the right thing to do will be to take linear combinations of the states in the degenerate subspace that set all $V_{nk} = 0$ for $n \neq k$. $\longleftarrow$ Diagonalize this operator in the subspace!

To be definite
g-fold degeneracy.

$\overbrace{— \; — \; — \; —}$ $\longleftarrow$ $E_D^{(0)}$ $\{|m^{(0)}\rangle\}$ $\xrightarrow{\lambda \to 0}$ $\{|\ell\rangle\}$

Unperturbed system.

As $\lambda \to 0$ $\{|\ell\rangle\} \to \{|\ell^{(0)}\rangle\} \neq \{|m^{(0)}\rangle\}$

Will be linear combinations

So how are $\{|\ell^{(0)}\rangle\}$ and $\{|m^{(0)}\rangle\}$ related?

$$|\ell^{(0)}\rangle = \sum_{m \in D} |m^{(0)}\rangle\langle m^{(0)}|\ell^{(0)}\rangle$$ Sum over the degenerate subspace.

Going back to the original Schrödinger Eq.

$\mathbb{P}_0$ = projection operator onto $\{|m^{(0)}\rangle\} = D$.

$\mathbb{P}_1 = \mathbb{1} - \mathbb{P}_0$; Note $\mathbb{1} = \mathbb{P}_0 + \mathbb{P}_1$

Then $(H_0 + \lambda V)|\ell\rangle = E|\ell\rangle$ or

just inserting the identity.

$$0 = (E - H_0 - \lambda V)|\ell\rangle = (E - H_0 - \lambda V)(\mathbb{P}_0 + \mathbb{P}_1)|\ell\rangle$$

$$0 = (E - E_D^{(0)} - \lambda V)\mathbb{P}_0|\ell\rangle + (E - H_0 - \lambda V)\mathbb{P}_1|\ell\rangle$$

Note here that $H_0\mathbb{P}_0|\ell\rangle = E_D^{(0)}\mathbb{P}_0|\ell\rangle$ because $\mathbb{P}_0|\ell\rangle \in D$ and <u>all</u> states in the degenerate subspace are energy eigenstates of H_0 with eigenvalue $E_D^{(0)}$.

Now, break this last result up into 2 parts by projecting out to kets in D and kets <u>not</u> in D. (Using $\mathbb{P}_0$ and $\mathbb{P}_1$).

Acting w/ $\mathbb{P}_0$ on the left: Recall $\mathbb{P}^2 = \mathbb{P}$ for a projection operator.

$$\boxed{0 = (E - E_D^{(0)} - \lambda\mathbb{P}_0 V)\mathbb{P}_0|\ell\rangle - \lambda\mathbb{P}_0 V\mathbb{P}_1|\ell\rangle}$$

Here we had $\mathbb{P}_0(E - H_0)\mathbb{P}_1$

$$= (E - H_0)\underbrace{\mathbb{P}_0\mathbb{P}_1}_{0}$$

Acting with $\mathbb{P}_1$ on the left:

$$\boxed{0 = -\lambda \mathbb{P}_1 V \mathbb{P}_0 |\ell\rangle + (E - H_0 - \lambda \mathbb{P}_1 V)\mathbb{P}_1 |\ell\rangle}$$

We can solve the 2nd equation in the subspace that is the orthogonal compliment to D.

$$\lambda \mathbb{P}_1 V \mathbb{P}_0 |\ell\rangle = (E - H_0 - \lambda \mathbb{P}_1 V)\mathbb{P}_1 |\ell\rangle \quad \text{or inverting}$$

$$\left[\mathbb{P}_1 (E - H_0 - \lambda V)\mathbb{P}_1\right]^{-1} = \mathbb{P}_1 \left[\frac{1}{E - H_0 - \mathbb{P}_1 \lambda V \mathbb{P}_1}\right]$$

project out in the orthogonal compliment $= \mathbb{P}_1$

a nonsingular operator in the $\mathbb{P}_1$ space since the eigenvalues of H_0 are not close to E in this subspace!

$$\Longrightarrow \boxed{\mathbb{P}_1 |\ell\rangle = \mathbb{P}_1 \frac{\lambda}{E - H_0 - \mathbb{P}_1 \lambda V \mathbb{P}_1} \mathbb{P}_1 V \mathbb{P}_0 |\ell\rangle}$$

<u>Now</u>, if we expand: $|\ell\rangle = |\ell^{(0)}\rangle + \lambda |\ell^{(1)}\rangle + \cdots$ and match terms order by order:

$$\mathbb{P}_1 |\ell^{(1)}\rangle = \sum_{m,\, k \notin D} |k^{(0)}\rangle\langle k^{(0)}| \frac{1}{E_D^{(0)} - H_0} |m^{(0)}\rangle\langle m^{(0)}| V \mathbb{P}_0 |\ell^{(0)}\rangle$$

plus $\mathcal{O}(\lambda)$ corrections.

$\mathbb{P}_1 =$ unperturbed states <u>not</u> in the degenerate space D.

dropping the order λ term here.

Already in the degenerate subspace!

So $$\mathbb{P}_1 |l^{(1)}\rangle = \sum_{k \notin D} |k^{(0)}\rangle \frac{1}{E_D^{(0)} - E_k^{(0)}} \langle k^{(0)}|V|l^{(0)}\rangle$$

This gives the part of the ket correction that is outside the degenerate subspace.

But we still need to figure out what is $|l^{(0)}\rangle$?

Go back to our first expression

$$(E - E_D^{(0)} - \lambda \mathbb{P}_0 V)\mathbb{P}_0 |l\rangle - \lambda \mathbb{P}_0 V \mathbb{P}_1 |l\rangle = 0$$

and plug in: $\mathbb{P}_1 |l\rangle = \mathbb{P}_1 \frac{\lambda}{E - H_0 - \lambda \mathbb{P}_1 V \mathbb{P}_1} \mathbb{P}_1 V \mathbb{P}_0 |l\rangle$

to get:

$$\left(E - E_D^{(0)} - \lambda \mathbb{P}_0 V \mathbb{P}_0 - \lambda^2 \mathbb{P}_0 V \mathbb{P}_1 \frac{1}{E - H_0 - \lambda \mathbb{P}_1 V \mathbb{P}_1} \mathbb{P}_1 V \mathbb{P}_0\right)|l\rangle = 0$$

collecting terms and recalling that $\mathbb{P}_1^2 = \mathbb{P}_1$ and $\mathbb{P}_0^2 = \mathbb{P}_0$

$$\left(E - E_D^{(0)} - \lambda \mathbb{P}_0 V \mathbb{P}_0 - \lambda^2 \mathbb{P}_0 V \mathbb{P}_1 \frac{1}{E - H_0 - \lambda V} \mathbb{P}_1 V \mathbb{P}_0\right) \mathbb{P}_0 |l\rangle = 0$$

watch out! here since the denominator is order λ, this term will matter at order λ, not λ^2 as you might think. But this will be a correction to $\mathbb{P}_0|l\rangle$ at order λ and not to the energies.

To lowest order the energies are given by:

$$\left(E - E_D^{(0)} - \lambda \mathbb{P}_0 V \mathbb{P}_0\right)\mathbb{P}_0|\ell^{(0)}\rangle = 0$$

$\uparrow$

$\lambda\Delta_\ell^{(1)} \leftarrow$ To 1^{st} order in λ

If we define $\mathbb{V} \leftarrow V$ matrix when restricted to $\mathbb{P}_0$ i.e. the matrix representation of $\mathbb{P}_0 V \mathbb{P}_0$ operator, we have

$$(\mathbb{P}_0 V \mathbb{P}_0)\mathbb{P}_0|\ell^{(0)}\rangle = \Delta_\ell^{(1)}\mathbb{P}_0|\ell^{(0)}\rangle$$ in the $|m^{(0)}\rangle$ bases

$$\mathbb{V}\begin{pmatrix}\langle m_1^{(0)}|\ell^{(0)}\rangle \\ \langle m_2^{(0)}|\ell^{(0)}\rangle \\ \vdots \\ \langle m_j^{(0)}|\ell^{(0)}\rangle\end{pmatrix} = \Delta_\ell^{(1)}\begin{pmatrix}\langle m_1^{(0)}|\ell^{(0)}\rangle \\ \vdots \\ \langle m_j^{(0)}|\ell^{(0)}\rangle\end{pmatrix}$$

This is just an eigenvalue/eigenvector problem. The eigenvalues are the 1^{st} order energy shifts and the eigenvectors are the 0^{th} order state kets $|\ell^{(0)}\rangle$.

In the $|\ell^{(0)}\rangle$ basis then $\Delta_\ell^{(1)} = \langle \ell^{(0)}|V|\ell^{(0)}\rangle$ the energy shifts are just like what we had before, but note that in this basis the $\mathbb{V}$ matrix is diagonal as we had hoped – this takes care of our singular energy denominators.

The states outside of the degenerate subspace don't matter so far. But they will show up at higher orders in perturbation theory.

This will be the perturbation!

Now let's find $\mathbb{P}_0|\ell\rangle$ to $\mathcal{O}(\lambda)$. We have to this order.

$$\Big(E - E_D^{(0)} - \underbrace{\lambda \mathbb{P}_0 V \mathbb{P}_0}_{\text{we will treat this as our bare Hamiltonian.}} - \lambda^2 \mathbb{P}_0 V \mathbb{P}_1 \frac{1}{E_D^{(0)} - H_0} \mathbb{P}_1 V \mathbb{P}_0 \Big) \mathbb{P}_0 |\ell\rangle = 0$$

needed only to order λ^0

Recall we have already solved the $g \times g$ eigenvalue problem. The eigenvalues of $\mathbb{P}_0 V \mathbb{P}_0 = \mathbb{V}$ are v_i, $i = 1, \ldots, g$. and the corresponding eigenvectors are $|\ell_i^{(0)}\rangle$, $i = 1, \ldots, g$.

$\Rightarrow$ The energies to 1st order are $E_i = E_D^{(0)} + \lambda v_i$

We will assume that all the v_i's are different so we can now apply <u>nondegenerate perturbation theory</u> to the $g \times g$ dimensional Hamiltonian above:

For that problem we found $|n^{(1)}\rangle = \sum_{k \neq n} \frac{|k\rangle V_{kn}}{E_n^{(0)} - E_k^{(0)}}$

Let's apply that result here:

$$\mathbb{P}_0 |\ell_i^{(1)}\rangle = \lambda \sum_{k \neq i} \frac{\mathbb{P}_0 |\ell_k^{(0)}\rangle}{v_i - v_k} \langle \ell_k^{(0)} | \mathbb{P}_0 V \mathbb{P}_1 \frac{1}{E_D^{(0)} - H_0} \mathbb{P}_1 V \mathbb{P}_0 | \ell_i^{(0)}\rangle$$

note the extra λ from λ^2/λ

We can simplify this a bit since $|\ell_i^{(0)}\rangle \in \mathbb{P}_1$ for all i

$$\mathbb{P}_0 |\ell_i^{(1)}\rangle = \lambda \sum_{k \neq i} \frac{\mathbb{P}_0 |\ell_k^{(0)}\rangle}{\upsilon_k - \upsilon_i} \langle \ell_j^{(0)} | V \mathbb{P}_1 \frac{1}{E_D^{(0)} - H_0} \mathbb{P}_1 V | \ell_i^{(0)}\rangle$$

$$\mathbb{P}_0 |\ell_i^{(1)}\rangle = \sum_{k \neq i} \frac{\lambda |\ell_k^{(0)}\rangle}{\upsilon_k - \upsilon_i} \sum_{p \notin D} \langle \ell_j^{(0)} | V | p\rangle \frac{1}{E_D^{(0)} - E_p^{(0)}} \langle p | V | \ell_i^{(0)}\rangle$$

from $\mathbb{P}_1$ Here you see the kets <u>not</u> in the degenerate subspace begin to matter.

Now $|\ell_i^{(1)}\rangle = \mathbb{P}_0 |\ell_i^{(1)}\rangle + \mathbb{P}_1 |\ell_i^{(1)}\rangle$ ← we have to add together the parts that we computed separately.

As before we set $\langle \ell^{(0)} | \ell \rangle = 1$. Then

$\lambda \langle \ell^{(0)} | V | \ell \rangle = (E - E_D^{(0)}) \langle \ell^{(0)} | \ell \rangle = \Delta_\ell$ or

$\Delta_\ell = \lambda \langle \ell^{(0)} | V | \ell \rangle$. Now, expand in λ as usual!

Thus : $\Delta_\ell^{(2)} = \langle \ell^{(0)} | V \mathbb{P}_1 | \ell^{(1)} \rangle + \langle \ell^{(0)} | V \mathbb{P}_0 | \ell^{(1)} \rangle$

recall that $\mathbb{P}_0 |\ell_j^{(0)}\rangle$ are eigenvectors of V the correction $\mathbb{P}_0 |\ell_j^{(1)}\rangle$ must be orthogonal to $\mathbb{P}_0 |\ell_j^{(0)}\rangle$ and thus the second matrix element vanishes — V is diagonal in this basis so $$\Delta_\ell^{(2)} = \sum_{k \notin D} \frac{|V_{k\ell}|^2}{E_D^{(0)} - E_k^{(0)}}$$

For summary:

1. Find the degenerate subspace and create the $g \times g$ perturbation matrix $\mathbb{V}$

2. Diagonalize $\mathbb{V}$

3. eigenvalues are energy shifts to 1st order and eigenvectors are the correct 0th order eigenkets.

4. At higher order use the nondegenerate results except now all summations exclude the <u>whole</u> degenerate subspace.