Degenerate Perturbation Theory

Reference: Griffiths Section 7.2, 7.3

Our first order formulas for perturbation theory are:

$E_n = E_n^0 + E_n^1$ $\qquad \hat{H} = \hat{H}^0 + \hat{H}^1$ $\qquad |\psi_n\rangle = |\psi_n^0\rangle + |\psi_n^1\rangle$

$$E_n^1 = \langle \psi_n^0 | \hat{H}^1 | \psi_n^0 \rangle$$

$$|\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^0 | \hat{H}^1 | \psi_n^0 \rangle}{(E_n^0 - E_m^0)} |\psi_m^0\rangle$$

In deriving this result, we assumed that $|\psi_n^0\rangle \neq |\psi_m^0\rangle$

$$(*) \quad \langle \psi_m^0 | \hat{H}^1 | \psi_n^0 \rangle = (E_n^0 - E_m^0)\langle \psi_m^0 | \psi_n^1 \rangle + \cancel{E_n^1 \delta_{n,m}}^{\,0}$$

What if there is some degeneracy so that $|\psi_m^0\rangle$ and $|\psi_n^0\rangle$ are orthogonal states with the <u>same</u> energy?

Notice that if $E_n^0 = E_m^0$, the denominator of $|\psi_n^1\rangle$ goes to zero, which is indicative of a problem.

We need to think more carefully about degenerate states...

Let's focus on the case of a twofold degeneracy to start. It is not hard to generalize it later.

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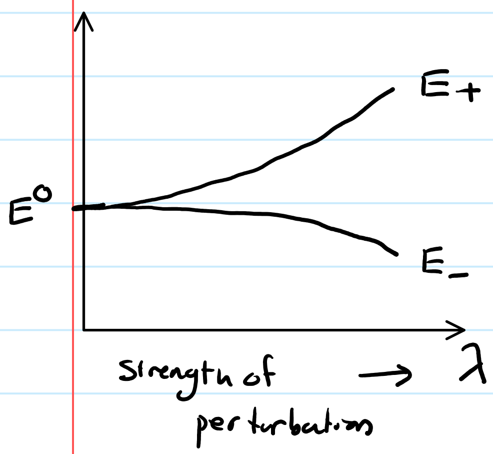
We suppose there are two states $|\phi_a^0\rangle$ and $|\phi_b^0\rangle$ which are degenerate in the absence of a perturbation.

$$\hat{H}^0|\phi_a^0\rangle = E^0|\phi_a^0\rangle \qquad \hat{H}^0|\phi_b\rangle = E^0|\phi_b^0\rangle$$

In the presence of a perturbation, we want to find corrections to the states and the energies with the understanding that the degeneracy will usually "lift" or "break" the degeneracy.



The "true" eigenstates will satisfy

$$\hat{H}|\psi_+\rangle = E_+|\psi_+\rangle$$
$$\hat{H}|\psi_-\rangle = E_-|\psi_-\rangle$$

And we seek to approximate

$$|\psi_+\rangle = |\psi_+^0\rangle + \lambda|\psi_+^1\rangle + \dots$$
$$|\psi_-\rangle = |\psi_-^0\rangle + \lambda|\psi_-^1\rangle + \dots$$
$$E_+ = E^0 + \lambda E_+^1 + \dots$$
$$E_- = E^0 + \lambda E_-^1 + \dots$$

Proceed as before; by expanding in powers of λ.

$$\hat{H}^0|\psi_+^1\rangle + \hat{H}^1|\psi_+^0\rangle = E^0|\psi_+^1\rangle + E_+^1|\psi_+^0\rangle$$

Now, comes the difference. In non-degenerate perturbation theory, we took the inner product with the state $\langle\psi^0|$ to get the energy correction. This was the eigenstate with energy E^0. But now, we have two such states. So, I could multiply by $\langle\phi_a^0|$ or $\langle\phi_b^0|$

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First order correction to energy for degenerate states

You might be thinking "why not just multiply by $\langle \psi_+^0 |$" then we'd get the same formula as before $E_+^1 = \langle \psi_+^0 | \hat{H}^1 | \psi_+^0 \rangle$

The problem is that I don't know what $|\psi_+^0\rangle$ is!

$|\psi_+^0\rangle \equiv$ the true eigenstate $|\psi_+\rangle$ in the limit when the perturbation is switched off.

All we know, right now is that $|\phi_a^0\rangle$ and $|\phi_b^0\rangle$ are degenerate eigenstates when $\lambda \to 0$, but any combination of these could be $|\psi_+^0\rangle$. How can we find the "good" combination?

Let's assume $|\psi_+^0\rangle = \alpha|\phi_a^0\rangle + \beta|\phi_B^0\rangle$ and our new goal is to find α and β. If I knew them, I'd know $|\psi_+^0\rangle$ and we could go back and safely use non-degenerate perturbation theory with this state.

$$\hat{H}^0|\psi_+^1\rangle + \hat{H}^1|\psi_+^0\rangle = E^0|\psi_+^1\rangle + E_+^1|\psi_+^0\rangle$$

multiply by $\langle \phi_a^0|$

$$\underbrace{\langle \phi_a^0|\hat{H}^0|\psi_+^1\rangle} + \langle \phi_a^0|\hat{H}^1|\psi_+^0\rangle = E^0\langle \phi_a^0|\psi_+^1\rangle + E_+^1\langle \phi_a^0|\psi_+^0\rangle$$

$= E^0\langle \phi_a^0|\psi_+^1\rangle$ as in non-degenerate theory. Cancels this

$$\langle \phi_a^0|\hat{H}^1|\psi_+^0\rangle = E_+^1\underbrace{\langle \phi_a^0|\psi_+^0\rangle} = E_+^1 \cdot \alpha$$

In non-degenerate theory, this was 1
Because there was only 1 state with energy E^0

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1 $\langle \phi_a^0 | \hat{H}' | \psi_+^0 \rangle = E_+^1 \alpha$

similarly, if we use $\langle \phi_b^0 |$ instead, we get

2 $\langle \phi_b^0 | \hat{H}' | \psi_+^0 \rangle = E_+^1 \beta$

Now sub in $|\psi_+^0\rangle = \alpha |\phi_a^0\rangle + \beta |\phi_b^0\rangle$

1 $\alpha \langle \phi_a^0 | \hat{H}' | \phi_a^0 \rangle + \beta \langle \phi_a^0 | \hat{H}' | \phi_b^0 \rangle = E_+^1 \alpha$

2 $\alpha \langle \phi_b^0 | \hat{H}' | \phi_a^0 \rangle + \beta \langle \phi_b^0 | \hat{H}' | \phi_b^0 \rangle = E_+^1 \beta$

Write this as matrices:

$$\underbrace{\begin{pmatrix} \langle \phi_a^0 | \hat{H}' | \phi_a^0 \rangle & \langle \phi_a^0 | \hat{H}' | \phi_b^0 \rangle \\ \langle \phi_b^0 | \hat{H}' | \phi_a^0 \rangle & \langle \phi_b^0 | \hat{H}' | \phi_b^0 \rangle \end{pmatrix}}_{\text{matrix representation of } \hat{H}' \text{ in the basis}} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E_+^1 \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$|\phi_a^0\rangle \rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\qquad |\phi_b^0\rangle \rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$|\psi_+^0\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$

so this matrix equation is just:

$$\boxed{\hat{H}' |\psi_+^0\rangle = E_+^1 |\psi_+^0\rangle}$$

In other words, E_+^1 is the eigenvalue of $\hat{H}'$ and the "good" state $|\psi_+^0\rangle$ is the corresponding eigenvector.

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Let's summarize...

Suppose you know two degenerate eigenstates $|\psi_a^0\rangle$, $|\psi_b^0\rangle$ and you want to know the "good combinations" of these, called $|\psi_+^0\rangle, |\psi_-^0\rangle$

and their first order energy corrections E_+^1, E_-^1.

1. Use the states $|\psi_a^0\rangle$, $|\psi_b^0\rangle$ as a basis
2. Find the matrix representation of $\hat{H}'$ in this basis.
3. Find its eigenvalues (E_+^1, E_-^1)
4. " " eigenvectors (ψ_+^0, ψ_-^0).

Put another way, we're looking for a basis of degenerate states $|\psi_+^0\rangle$, $|\psi_-^0\rangle$ in which $\hat{H}'$ is diagonal. Then, the energy corrections lie on the diagonal

$$\hat{H}' \xrightarrow{\text{"good basis"}} \begin{pmatrix} E_-^1 & 0 \\ 0 & E_+^1 \end{pmatrix}$$

Once $|\psi_+^0\rangle$ and $|\psi_-^0\rangle$ are known, we can go back and use <u>non-degenerate</u> perturbation theory!

<u>Take-Home Message</u>: When doing perturbation theory with degenerate states, always work in a basis of degenerate states in which $\hat{H}'$ is diagonal. Then, you'll have no problems!