Physics 137B Lecture 8

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1 February 2 - Degenerate Perturbation Theory Continued

Recap

- Last time we considered a system with two-fold degeneracy i.e. two orthonormal states ψ_a, ψ_b with the same energy E. The energies being the same causes our formula for the first-order correction obtained in non-degenerate PT to diverge.
- However, we found that if we consider linear combinations of the degenerate states $|\Psi\rangle_{\pm} = \alpha |\psi_a\rangle + \beta |\psi_b\rangle$ and solve the eigenvalue problem

$$\mathbf{W} \cdot \tilde{\mathbf{V}} = E^{(0)} \tilde{\mathbf{V}}$$

where

$$\mathbf{W} = \begin{pmatrix} H'_{aa} & H'_{ab} \\ H'_{ba} & H'_{bb} \end{pmatrix}$$

then we obtain α, β such that $|\Psi\rangle_{\pm}$ diagonalize the degenerate subspace and allow us to lift the degeneracy.

• We saw an example in the 2D Harmonic Oscillator, where we wrote the unperturbed hamiltonian in terms of raising and lowering operators as

$$\hat{H}_0 = \hbar\omega \left(\hat{a}_+ \hat{a}_- + \hat{b}_+ \hat{b}_- + 1 \right)$$

and then introduced the perturbation

$$\hat{H}' = \lambda m \omega^2 \hat{x} \hat{y}$$

• We were able to solve this problem exactly by changing to *normal coordinates* and found the energy to be

$$E_{nn'} = \left(n + \frac{1}{2}\right)\hbar\omega\left(1 + \lambda\right)^{1/2} + \left(n' + \frac{1}{2}\right)\hbar\omega\left(1 - \lambda\right)^{1/2}$$

Today, we will solve for the first order correction using Perturbation Theory and check that it agrees with the exact solution.

1.1 Perturbation Theory approach to 2D Harmonic Oscillator

• The perturbation $\hat{H}' = \lambda m\omega^2 \hat{x}\hat{y}$ can be written in terms of the raising and lowering operators as

$$\hat{H}' = \frac{\lambda \hbar \omega}{2} \left(\hat{a}_+ + \hat{a}_- \right) \left(\hat{b}_+ + \hat{b}_- \right)$$

• The unperturbed solutions can be written as

$$|n, n'\rangle^{(0)} = |n^{(0)}\rangle_a \otimes |n'\rangle_b^{(0)}$$
$$= \frac{(\hat{a}_+)^n}{\sqrt{n!}} \frac{(\hat{b}_+)^{n'}}{\sqrt{(n')!}} |00\rangle^{(0)}$$

where $|00\rangle^{(0)}$ is the unperturbed ground state.

• These are all the tools we need to approach the problem. Let's now calculate the first order energy correction to the first excited state.

Let's get to evaluating the W matrix.

$$\mathbf{W} = \begin{pmatrix} \langle 10|\hat{H}'|10\rangle & \langle 10|\hat{H}'|01\rangle \\ \langle 01|\hat{H}'|10\rangle & \langle 01|\hat{H}'|01\rangle \end{pmatrix}$$

The algebra here seems tedious but we can notice that the perturbation contains raising and lowering operators, which means the diagonal elements are all going to be zero.

Further,

$$\hat{H}'|10\rangle = \frac{\hbar\omega}{2} \left(\hat{a}_{+} + \hat{a}_{-}\right) \left(\hat{b}_{+} + \hat{b}_{-}\right) |10\rangle$$

$$= \frac{\hbar\omega}{2} \left(\hat{b}_{+} + \hat{b}_{-}\right) \left(\sqrt{2}|20\rangle + |00\rangle\right)$$

$$= \frac{\hbar\omega}{2} \left(\sqrt{2}|21\rangle + |01\rangle\right)$$

So,

$$\langle 10|\hat{H}'|10\rangle = 0$$
$$\langle 01|\hat{H}'|10\rangle = \frac{\hbar\omega}{2}$$

Calculating the other column values, we find

$$\mathbf{W} = \frac{\hbar\omega}{2} \begin{pmatrix} 0 & 1\\ 1 & 0 \end{pmatrix}$$

Now that we've found \mathbf{W} , we can find the first-order energy corrections:

$$\begin{split} E_0^{(1)} &= \frac{1}{2} \left[H'_{aa} + H'_{bb} + \sqrt{(H'_{aa} - H'_{bb}) + 4|E'_{ab}|^2} \right] \\ &= \pm \frac{1}{2} \sqrt{4 \cdot \left(\frac{\hbar \omega}{2}\right)^2} \\ &= \pm \frac{\hbar \omega}{2} \lambda \end{split}$$

So the energy corrections to the first excited state are

$$E_{\pm}^{(1)} = \pm \frac{\hbar\omega}{2}\lambda$$

Let's now compare this result to the exact solution, which is given by

$$E_{nn'} = \left(n + \frac{1}{2}\right)\hbar\omega \left(1 + \lambda\right)^{1/2} + \left(n' + \frac{1}{2}\right)\hbar\omega \left(1 - \lambda\right)^{1/2}$$

So, the exact $|01\rangle$ energy is

$$\begin{split} E_{0,1} &= \left(0 + \frac{1}{2}\right) \hbar \omega \underbrace{\left(1 + \lambda\right)^{1/2}}_{=\left(1 + \frac{\lambda}{2} + \cdots\right)} + \left(1 + \frac{1}{2}\right) \hbar \omega \underbrace{\left(1 - \lambda\right)^{1/2}}_{=\left(1 - \frac{\lambda}{2} + \cdots\right)} \\ &= \left(0 + \frac{1}{2} + 1 + \frac{1}{2}\right) \hbar \omega + \lambda \left(\frac{1}{4} - \frac{1}{2} - \frac{1}{4}\right) \hbar \omega + \mathcal{O}(\lambda^2) \\ &\approx \underbrace{2\hbar \omega}_{=E_{01}^{(0)}} - \underbrace{\frac{\hbar \omega}{2} \lambda}_{E_{01,(-)}^{(1)}} \end{split}$$

and this matches up with the result we using the **W** matrix. Similarly, we can check that the results match up for the $|10\rangle$ energy correction, or more generally the $|n, n'\rangle$ correction.

For the $|n, n'\rangle$ case, we have

$$E_{n,n'} = \left(n + \frac{1}{2}\right)\hbar\omega\underbrace{\left(1 + \lambda\right)^{1/2}}_{=\left(n' + \frac{\lambda}{2} + \cdots\right)} + \left(1 + \frac{1}{2}\right)\hbar\omega\underbrace{\left(1 - \lambda\right)^{1/2}}_{=\left(1 - \frac{\lambda}{2} + \cdots\right)}$$

$$= \left(n + \frac{1}{2} + n' + \frac{1}{2}\right)\hbar\omega + \lambda\left(\frac{n}{2}\frac{1}{4} - \frac{n'}{2} - \frac{1}{4}\right)\hbar\omega + \mathcal{O}(\lambda^2)$$

$$\approx \underbrace{\left(n + n' + 1\right)\hbar\omega}_{=E_{n,n'}^{(0)}} - \underbrace{\left(n - n'\right)\frac{\hbar\omega}{2}\lambda}_{E_{n,n'}^{(1)}}$$

Note: If the states $|a\rangle, |b\rangle$ are degenerate but still give us a **W** matrix whose off diagonals are trivial,

$$\mathbf{W} = \begin{pmatrix} H'_{aa} & 0 \\ 0 & H'_{bb} \end{pmatrix}$$

then the eigenvalue problem is solved by default! The $|a\rangle$ -state energy correction and the $|b\rangle$ -state energy correction are simply H'_{aa} and H'_{bb}

$$E_a^{(1)} = H'_{aa}$$
$$E_b^{(1)} = H'_{bb}$$

In other words, the basis we started off with was already the "good" basis! We didn't need to solve the Eigenvalue problem to find a different degenerate-eigenspace-basis to diagonalize it.

1.2 Good States

Theorem: If $|a\rangle, |b\rangle$ are degenerate with respect to \hat{H} and there exists a hermitian operator \hat{A} such that

1. The states $|a\rangle,|b\rangle$ are eigenstates of \hat{A} with distinct eigenvalues $(a\neq b)$

$$\hat{A}|a\rangle=a|a\rangle$$

$$\hat{A}|b\rangle = b|b\rangle$$

and \hat{A} commutes with the unperturbed hamiltonian as well as the perturbation,

2.

$$[\hat{A}, \hat{H}'] = [\hat{A}, \hat{H}_0] = [\hat{A}, \hat{H}] = 0$$

then the eigenvectors of \hat{A} form a "good basis" to use in the perturbation theory.

Proof: Let $\hat{H}(\lambda) = \hat{H}_0 + \lambda \hat{H}'$ and \hat{A} commute. [Finish later]