PHYS 487: Lecture # 8

Cliff Sun

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Lecture Span

- Degenerate perturbation theory

Lecture recap

We expanded the wavefunction and energies in a power series

$$|\psi_n\rangle = \sum_{i=0} \lambda^i \left|\psi_n^{(i)}\right\rangle$$
$$E_n = \sum_{i=0} \lambda^i E_n^{(i)}$$

Then we found that

$$E_n^{(1)} = \langle\psi_n^{(0)}|H'|\psi_n^{(0)}\rangle \tag{1}$$
$$\left|\psi_n^{(1)}\right\rangle = \sum_{m\neq n} \frac{\langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} \tag{2}$$

But now, what do we do if there is a degeneracy?

Degenerate perturbation theory

$$\left|\psi_n^{(1)}\right\rangle = \sum_{m\neq n} \frac{\langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} \tag{3}$$

But what if $E_m^{(0)} = E_n^{(0)}$. Q: can we guarantee $\langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle = 0$?

Example: Two-fold degeneracy

Let there be two eigenstates $|\psi_a\rangle$ and $|\psi_b\rangle$. And given

$$H^{(0)}\left|\psi_i^{(0)}\right\rangle = E^{(0)}\left|\psi_i^{(0)}\right\rangle$$
$$\langle\psi_i|\psi_k\rangle = \delta_{ik}$$

Moreover, any $\alpha\left|\psi_a^{(0)}\right\rangle + \beta\left|\psi_b^{(0)}\right\rangle \equiv |\psi^{(0)}\rangle$. With the following:

$$H^{(0)}\left|\psi^{(0)}\right\rangle = E^{(0)}\left|\psi^{(0)}\right\rangle \tag{4}$$

We note that $|\psi_a\rangle$ and $|\psi_b\rangle$ are degenerate. And combining them into $|\psi\rangle$ also yields the same energy. Because you get a constant $E^{(0)}$ out in front of them.

Idea: Find eigenstates of H'; $H = H^{(0)} + \lambda H'$, and $\lim_{\lambda\to 0} H$ is good states.

Example

$$H^{(0)} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x^2+y^2\right) \tag{5}$$

Consider the first excited state:

$$|\psi_a\rangle = \psi_0(x)\psi_1(y) = \sqrt{\frac{2}{\pi}}\frac{m\omega}{\hbar}ye^{-\frac{m\omega}{2\hbar}\left(x^2+y^2\right)} \equiv |0_x, 1_y\rangle \tag{6}$$

and

$$|\psi_b\rangle = \psi_1(x)\psi_0(y) = \sqrt{\frac{2}{\pi}}\frac{m\omega}{\hbar}ye^{-\frac{m\omega}{2\hbar}\left(x^2+y^2\right)} \equiv |1_x, 0_y\rangle \tag{7}$$

Consider a perturbation $H' = \epsilon m\omega^2 xy$. Then if x, y are the same sign, then $\langle H'\rangle > 0$. But if x, y are different signs, then $\langle H'\rangle < 0$. Here, the perturbation then corrects (or "lifts") the degeneracy of the system.

Next, introduce

$$x' = \frac{x+y}{\sqrt{2}}, \quad y' = \frac{x-y}{\sqrt{2}} \tag{8}$$

Then

$$H = \frac{p^2}{2m} + \frac{m}{2}\left(1+\epsilon\right)\omega^2 x'^2 + \frac{m}{2}\left(1-\epsilon\right)\omega^2 y'^2 \tag{9}$$

This is just two uncoupled harmonic oscillators. Then we get

$$\psi_{mn} = \psi_m^+(x')\psi_n^-(y') \quad \omega_\pm = \sqrt{1\pm\epsilon}\omega \tag{10}$$

$$E_{mn} = \left(m+\frac{1}{2}\right)\hbar\omega_+ + \left(n+\frac{1}{2}\right)\hbar\omega_- \tag{11}$$

Then as $\epsilon \to 0$,

$$\psi_{01} = \psi_0\left(\frac{x+y}{\sqrt{2}}\right)\psi_1\left(\frac{x-y}{\sqrt{2}}\right) = \frac{-\psi_a^{(0)} + \psi_b^{(0)}}{\sqrt{2}} \tag{12}$$

Recipe for finding the good states

We first start with the λ^n equations. Next, we guess some states $|\psi_a\rangle$ and $|\psi_b\rangle$ that are degenerate in order to find "good" states such that

$$\left|\psi^{(0)}\right\rangle = \alpha\left|\psi_a^{(0)}\right\rangle + \beta\left|\psi_b^{(0)}\right\rangle \tag{13}$$

Then

$$H^{(0)}\left|\psi^{(0)}\right\rangle + \lambda(H'\left|\psi^{(0)}\right\rangle + H^{(0)}\left|\psi^{(1)}\right\rangle) = E^{(0)}\left|\psi^{(0)}\right\rangle + \lambda\left(E^{(1)}\left|\psi^{(0)}\right\rangle + E^{(0)}\left|\psi^{(1)}\right\rangle\right) \tag{14}$$

For λ^1 equation, we have that

$$H'\left|\psi^{(0)}\right\rangle + H^{(0)}\left|\psi^{(1)}\right\rangle = E^{(1)}\left|\psi^{(0)}\right\rangle + E^{(0)}\left|\psi^{(1)}\right\rangle \tag{15}$$

Multiply both sides by $\left\langle\psi_a^{(0)}\right|$:

$$\langle\psi_a^{(0)}|H^{(0)}|\psi^{(1)}\rangle + \langle\psi_a^{(0)}|H'|\psi^{(0)}\rangle = E^{(0)}\langle\psi_a^{(0)}|\psi^{(1)}\rangle + E^{(1)}\langle\psi_a^{(0)}|\psi^{(0)}\rangle \tag{16}$$

With $\alpha\left|\psi_a^{(0)}\right\rangle + \beta\left|\psi_b^{(0)}\right\rangle = \left|\psi^{(0)}\right\rangle$ and $\left\langle\psi_a^{(0)}\middle|\psi_b^{(0)}\right\rangle = 0$. Then, we get

$$\alpha\langle\psi_a^{(0)}|H'|\psi_a^{(0)}\rangle + \beta\langle\psi_a^{(0)}|H'|\psi_b^{(0)}\rangle = \alpha E^{(1)} \tag{17}$$

Repeat with $\left\langle\psi_b^{(0)}\right|$, then we get

$$\begin{pmatrix} w_{aa} & w_{ab} \\ w_{ba} & w_{bb} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E^{(1)} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \tag{18}$$

So then the eigenvalues of W are the energy corrections. And the eigenvectors are the "good" α and β. So then, we have solutions

$$E_{\pm}^{(1)} = \frac{1}{2}\left[w_{aa} + w_{bb} \pm \sqrt{(w_{aa} - w_{bb})^2 + 4|w_{ab}|^2}\right] \tag{19}$$

Theorem 0.1. *If A is hermitian and $[A, H^{(0)}] = 0 = [A, H']$. If $A\left|\psi_a^{(0)}\right\rangle = \mu\left|\psi_a^{(0)}\right\rangle$, $A\left|\psi_b^{(0)}\right\rangle = \gamma\left|\psi_b^{(0)}\right\rangle$ and $\mu \neq \gamma$. Then $|\psi_a\rangle$ and $|\psi_b\rangle$ are the good states for perturbation theory.*

Example

Here, $H^{(0)}$ is rotationally symmetric and H' is a discrete rotational symmetry. Then we cannot use the previous theorem where $\mu \neq \gamma$. Then,

Big takeaway

We study how degenerate states evolve with perturbation. So $\left|\psi^{(0)}\right\rangle$ really is a function of λ, so it changes to remain an "approximate" eigenstate of $H = H^{(0)} + \lambda H'$.