Physics 472 Lecture 11

1) Applications of nondegenerate perturbation theory: Anharmonic oscillators

i) Consider a perturbation of the simple harmonic oscillator,

$$H = H_0 + \lambda H_1 , \qquad H_0 = \frac{p_x^2}{2m} + \frac{m\omega^2 x^2}{2}$$

$$H_1 = b x^3$$

What is the lowest order correction to the ground-state energy?

$$E_0 = \frac{\hbar\omega}{2} + \lambda E_0^{(1)} + \lambda^2 E_0^{(2)} + \cdots$$

$$E_0^{(1)} = \langle 0 | b x^3 | 0 \rangle = 0 \quad \text{(why?)}$$

$$E_0^{(2)} = \sum_{n>0} \frac{|\langle n| bx^3 |0\rangle|^2}{E_0^{(0)} - E_n^{(0)}}$$

$$E_n^{(0)} = \hbar\omega(n + 1/2)$$

$$E_0^{(2)} = \frac{b^2}{\hbar\omega} \sum_{n>0} \frac{|\langle n|x^3|0\rangle|^2}{-n}$$

Now $\quad x = \sqrt{\frac{\hbar}{2m\omega}}\,(a + a^\dagger)$

and $\quad a|n\rangle = \sqrt{n}\,|n-1\rangle$

$$a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle .$$

$$x^3 = \left(\frac{\hbar}{2m\omega}\right)^{3/2}(a + a^\dagger)^3$$

$$(a+a^\dagger)^3 = a^3 + a^2 a^\dagger + a a^\dagger a + a^\dagger a^2 + a(a^\dagger)^2 + a^\dagger a a^\dagger + (a^\dagger)^2 a + (a^\dagger)^3$$

$$(a+a^\dagger)^3|0\rangle = \left[a(a^\dagger)^2 + a^\dagger a a^\dagger + (a^\dagger)^3\right]|0\rangle$$

$$= \sqrt{1\cdot 2\cdot 2}\,|1\rangle + 1\,|1\rangle + \sqrt{1\cdot 2\cdot 3}\,|3\rangle$$

$$= 3\,|1\rangle + \sqrt{6}\,|3\rangle$$

$$\langle 1|(a+a^\dagger)^3|0\rangle = 3$$

$$\langle 3|(a+a^\dagger)^3|0\rangle = \sqrt{6}$$

All other matrix elements vanish.

$$E_0^{(2)} = \frac{b^2}{\hbar\omega}\left(\frac{\hbar}{2m\omega}\right)^{3/2}\left[-9 - \frac{6}{3}\right]$$

$$E_0^{(2)} = -\frac{11\, b^2}{\hbar\omega}\left(\frac{\hbar}{2m\omega}\right)^{3/2}$$

Furthermore, the first-order correction to the ground state is

$$|\psi_0^{(1)}\rangle = \frac{|1\rangle\langle 1|\, bx^3\, |0\rangle}{E_0^{(0)} - E_1^{(0)}}$$

$$+ \frac{|3\rangle\langle 3|\, bx^3\, |0\rangle}{E_0^{(0)} - E_3^{(0)}}$$

$$= -\frac{b}{\hbar\omega}\left(\frac{\hbar}{2m\omega}\right)^{3/2}\left(3\,|1\rangle + \sqrt{\frac{2}{3}}\;|3\rangle\right)$$

$$|\psi_0\rangle \simeq |\psi_0^{(0)}\rangle + \lambda\,|\psi_0^{(1)}\rangle$$

contains admixture of states $|1\rangle$ and $|3\rangle$.

Setting $\lambda = 1$, we have

$$\psi_0(x) = \langle x | \psi_0 \rangle \simeq \langle x | \psi_0^{(0)} \rangle + \langle x | \psi_0^{(1)} \rangle$$

$$= \psi_0^{(0)}(x) + \psi_0^{(1)}(x)$$

$$= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\xi^2/2} \left[1 - \frac{b}{\hbar\omega}\left(\frac{\hbar}{2m\omega}\right)^{3/2}\left(\frac{\xi}{\sqrt{2}} + \frac{2\sqrt{2}}{3}\xi^3\right)\right]$$

where $\xi = \sqrt{\frac{m\omega}{\hbar}}\, x$.

ii) $H_1 = c x^4$

What is the lowest order correction to the energy of the nth eigenstate?

$$\Delta E_n^{(1)} = \langle n | H_1 | n \rangle$$

$$= c \langle n | x^4 | n \rangle$$

$$\Delta E_n^{(1)} = C\left(\frac{\hbar}{2m\omega}\right)^2 \langle n|(a+a^\dagger)^4|n\rangle$$

$$\begin{aligned}(a+a^\dagger)^4 &= \left(a^2+a^{\dagger 2}+aa^\dagger+a^\dagger a\right)^2 \\ &= \left(1+a^2+a^{\dagger 2}+2a^\dagger a\right)^2 \\ &= 1+a^2(a^\dagger)^2+(a^\dagger)^2a^2 \\ &\quad +4(a^\dagger a)^2+4a^\dagger a \\ &\quad + \text{off-diagonal terms}\end{aligned}$$

$$\Delta E_n^{(1)} = C\left(\frac{\hbar}{2m\omega}\right)^2\left(1+4n+4n^2 + \sqrt{(n+2)^2(n+1)^2} + \sqrt{n^2(n-1)^2}\right)$$

$$\Delta E_n^{(1)} = \frac{3C}{4}\left(\frac{\hbar}{m\omega}\right)^2\left(1+2n+2n^2\right)$$

$$\Delta E_0^{(1)} = \frac{3c}{4}\left(\frac{\hbar}{m\omega}\right)^2$$

$$\Delta E_1^{(1)} = \frac{15c}{4}\left(\frac{\hbar}{m\omega}\right)^2$$

$$\Delta E_2^{(1)} = \frac{39c}{4}\left(\frac{\hbar}{m\omega}\right)^2, \quad \text{etc.}$$

Does the sign of $\Delta E_n^{(1)}$ seem reasonable? Does the rapid increase of $\Delta E_n^{(1)}$ with n seem reasonable?

(ii) <u>Perturbations of a two-state system</u> Consider two states $|1\rangle$ + $|2\rangle$ with $H_0|1\rangle = \varepsilon_1|1\rangle$, $H_0|2\rangle = \varepsilon_2|2\rangle$.

In matrix form,

$$H_0 = \begin{pmatrix} \varepsilon_1 & 0 \\ 0 & \varepsilon_2 \end{pmatrix}.$$

$$H_1 = \begin{pmatrix} \langle 1|H_1|1\rangle & \langle 1|H_1|2\rangle \\ \langle 2|H_1|1\rangle & \langle 2|H_1|2\rangle \end{pmatrix}$$

The first-order corrections to the eigenenergies are

$$E_1^{(1)} = \langle 1|H_1|1\rangle, \quad E_2^{(1)} = \langle 2|H_1|2\rangle.$$

The second-order corrections are

$$E_1^{(2)} = \frac{|\langle 2|H_1|1\rangle|^2}{\varepsilon_1 - \varepsilon_2}$$

$$E_2^{(2)} = \frac{|\langle 2|H_1|1\rangle|^2}{\varepsilon_2 - \varepsilon_1} = -E_1^{(2)}$$

Suppose $\varepsilon_1 < \varepsilon_2$. Then E_1 is pushed down in second order, while E_2 is pushed up:

Setting $\lambda = 1$,

$$E_1 = \varepsilon_1 + \langle 1|H_1|1\rangle - \frac{|\langle 2|H_1|1\rangle|^2}{|\varepsilon_2 - \varepsilon_1|}$$

$$E_2 = \varepsilon_2 + \langle 2|H_1|2\rangle + \frac{|\langle 2|H_1|1\rangle|^2}{|\varepsilon_2 - \varepsilon_1|}$$

or

$$E_1 = \tilde{\varepsilon}_1 - \frac{|V|^2}{\varepsilon_2 - \varepsilon_1}$$

$$E_2 = \tilde{\varepsilon}_2 + \frac{|V|^2}{\varepsilon_2 - \varepsilon_1},$$

with $\langle 2|H_1|1\rangle \equiv V$ and

$$\tilde{\mathcal{E}}_i = \mathcal{E}_i + \langle i|H_1|i\rangle .$$

This phenomenon is known as "level repulsion."

There is a problem if $\mathcal{E}_2 \to \mathcal{E}_1$. Then the second-order corrections diverge, and perturbation theory fails! However, we can solve this two-level system exactly:

$$H = H_0 + H_1 = \begin{pmatrix} \tilde{\mathcal{E}}_1 & V \\ V^* & \tilde{\mathcal{E}}_2 \end{pmatrix}$$

The energy eigenvalues are determined by

$$\begin{vmatrix} \tilde{\varepsilon}_1 - \lambda & V \\ V^* & \tilde{\varepsilon}_2 - \lambda \end{vmatrix} = 0$$

$$(\tilde{\varepsilon}_1 - \lambda)(\tilde{\varepsilon}_2 - \lambda) - |V|^2 = 0$$

$$\lambda^2 - (\tilde{\varepsilon}_1 + \tilde{\varepsilon}_2)\lambda + \tilde{\varepsilon}_1 \tilde{\varepsilon}_2 - |V|^2 = 0$$

$$\lambda = \frac{\tilde{\varepsilon}_1 + \tilde{\varepsilon}_2}{2} \pm \sqrt{\left(\frac{\tilde{\varepsilon}_1 + \tilde{\varepsilon}_2}{2}\right)^2 - \tilde{\varepsilon}_1 \tilde{\varepsilon}_2 + |V|^2}$$

$$E_\pm = \frac{\tilde{\varepsilon}_1 + \tilde{\varepsilon}_2}{2} \pm \sqrt{\left(\frac{\tilde{\varepsilon}_1 - \tilde{\varepsilon}_2}{2}\right)^2 + |V|^2}$$

If we expand the exact energies to leading order in H_1, we find

$$E_\pm = \frac{\tilde{\varepsilon}_1 + \tilde{\varepsilon}_2}{2} \pm \frac{\tilde{\varepsilon}_2 - \tilde{\varepsilon}_1}{2}\left(1 + \left|\frac{2V}{\tilde{\varepsilon}_2 - \tilde{\varepsilon}_1}\right|^2\right)^{1/2}$$

$$E_\pm \cong \frac{\tilde{\varepsilon}_1 + \tilde{\varepsilon}_2}{2} \pm \frac{\tilde{\varepsilon}_2 - \tilde{\varepsilon}_1}{2} \pm \frac{|V|^2}{\tilde{\varepsilon}_2 - \tilde{\varepsilon}_1}$$

$$E_+ \cong \tilde{\varepsilon}_2 + \frac{|V|^2}{\tilde{\varepsilon}_2 - \tilde{\varepsilon}_1}$$

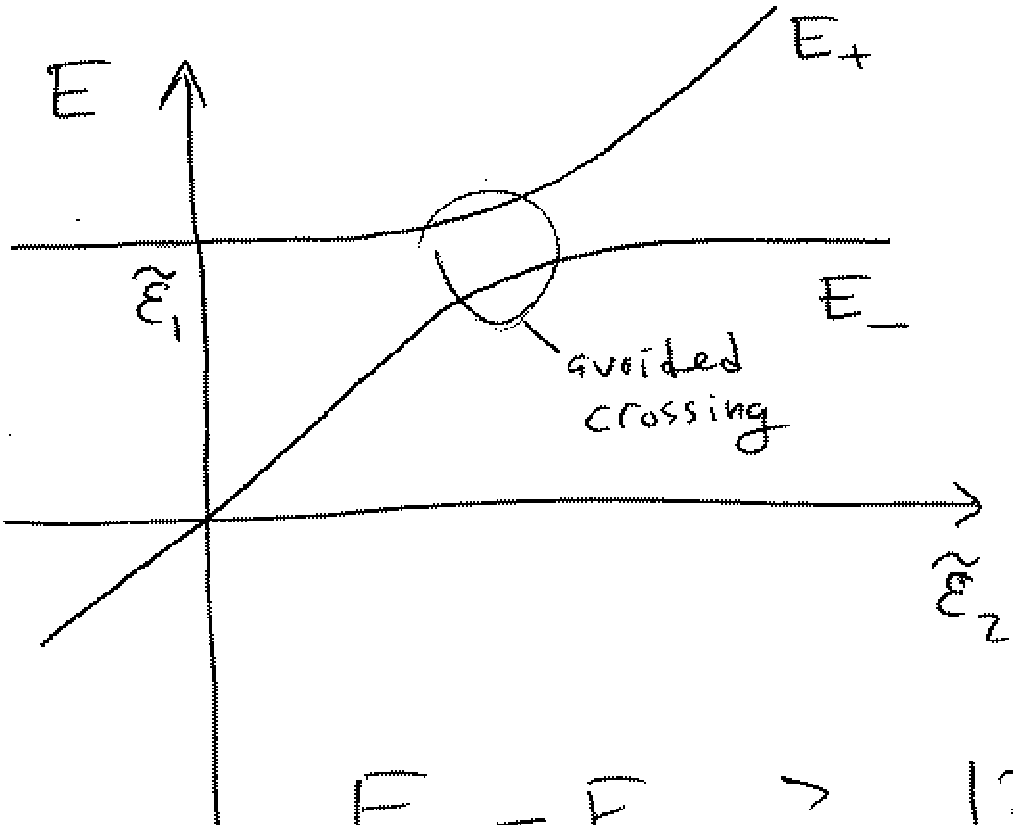
$$= \varepsilon_2 + \langle 2|H_1|2\rangle + \frac{|\langle 2|H_1|1\rangle|^2}{\varepsilon_2 - \varepsilon_1} + \mathcal{O}(H_1^3)$$

$$E_- = \varepsilon_1 + \langle 1|H_1|1\rangle - \frac{|\langle 2|H_1|1\rangle|^2}{\varepsilon_2 - \varepsilon_1} + \mathcal{O}(H_1^3)$$

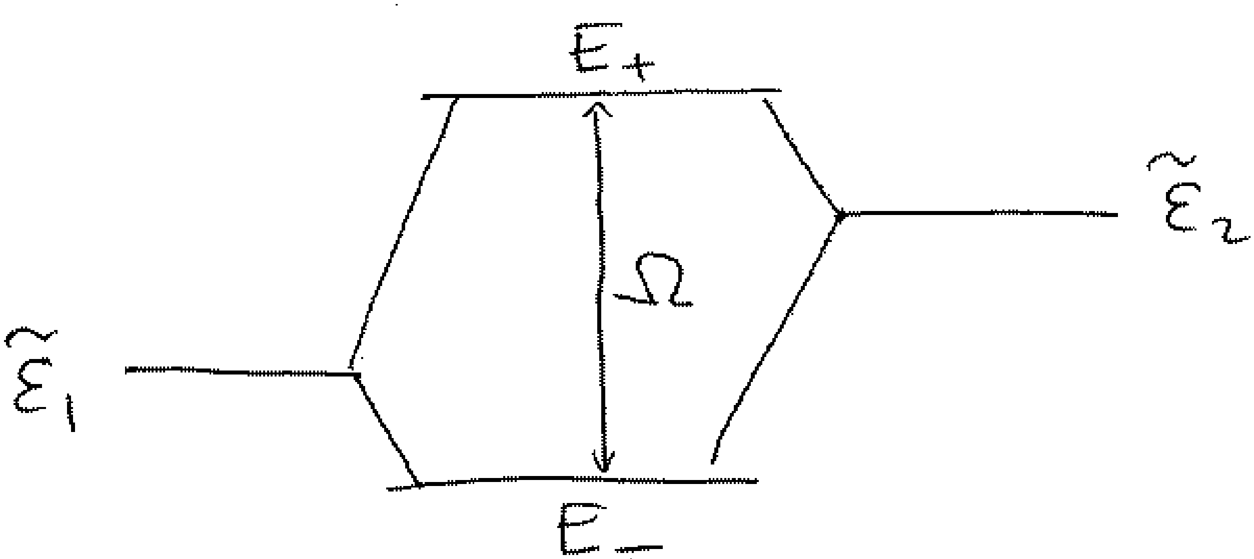
Thus we recover the perturbative results provided $\varepsilon_2 \neq \varepsilon_1$.

When $\varepsilon_1 = \varepsilon_2$, $H_0 = \varepsilon_1 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, and the problem reduces to that of diagonalizing H_1.

That is to say, if the eigenvalues of H_0 are <u>degenerate</u>, we can choose appropriate linear combinations of $|1\rangle$ and $|2\rangle$ that have the same eigenvalue with respect to H_0, but which also diagonalize H_1. This is the method of <u>degenerate perturbation theory</u>.



$$E_+ - E_- \geq |2V|$$



$$\Omega = \sqrt{(\tilde{\varepsilon}_2 - \tilde{\varepsilon}_1)^2 + 4|V|^2}$$