OPTI 570 LECTURE TU NOV 18

PERTURBATION THEORY

$$H = \underbrace{\frac{p^2}{2m} + \frac{1}{2} m\omega_0^2 (x^2+y^2)} + \hbar\omega\left(\frac{x}{6}\right)^4$$

Q: eigenvalues and eigenstates of H?

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega_0^2 (x^2+y^2)$$

w/ eigenstate basis $\{ |\varphi_n^i\rangle \}$

where $H_0 |\varphi_n^i\rangle = E_n |\varphi_n^i\rangle$

$E_n = \hbar\omega_0(n+1)$, $n = n_x + n_y$

$\{ |n_x, n_y\rangle \}$ written now $\{ |\varphi_n^i\rangle \}$

$|0,0\rangle = |\varphi_0\rangle$ - E_0

$|1,0\rangle = |\varphi_1^1\rangle$
$|0,1\rangle = |\varphi_1^2\rangle$ } both energy E_1

$|2,0\rangle = |\varphi_2^1\rangle$
$|1,1\rangle = |\varphi_2^2\rangle$ } all energy E_2
$|0,2\rangle = |\varphi_2^3\rangle$

...

$$H = H_0 + \hbar\omega\left(\frac{x}{6}\right)^4$$

Options:
- analythic solution, if possible (in general NOT)
- numerical / computational
- approximation methods

$$H = H_0 + \underbrace{\hbar\omega\left(\frac{x}{6}\right)^4}_{W}$$

<u>case</u>: W is small compared to H_0

$$H = H_0 + \underbrace{W}_{\text{small perturbation}}$$

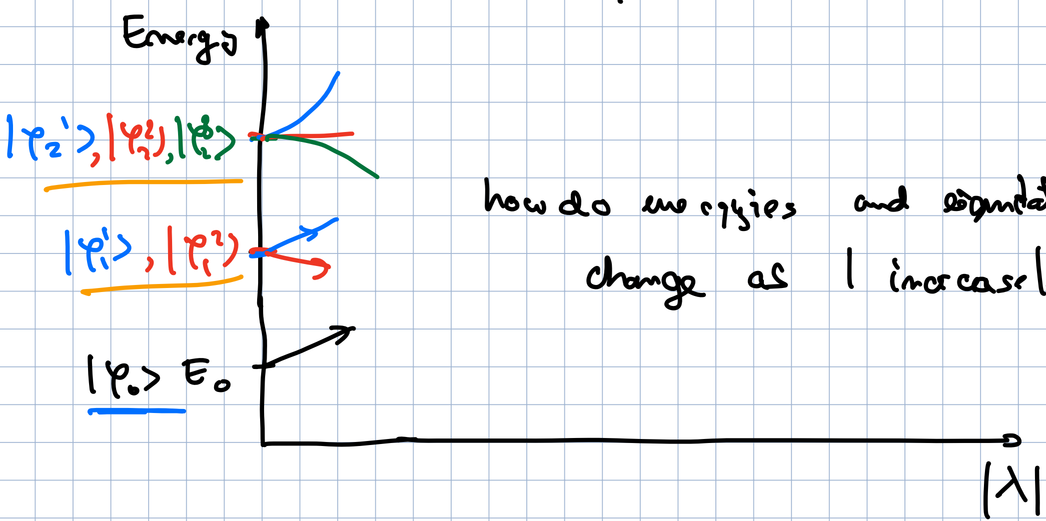
$$W = \hbar\,\omega\left(\frac{x}{6}\right)^4$$

$$W = \underbrace{\frac{\omega}{\omega_0}}\,\hbar\,\omega_0\left(\frac{x}{6}\right)^4 =$$

$$= \underset{\sim}{\lambda}\;\underbrace{\hbar\,\omega_0\left(\frac{x}{6}\right)^4}_{\hat{W}}$$

$$W = \underline{\lambda}\,\hat{W}$$

W - small $\Rightarrow$ $|\lambda| \ll 1$



how do energies and eigenstates change as | increase $|\lambda|$)

Stationary perturbation theory

(1) Non-degenerate : no degeneracies in H_0 $g_n = 1$

(2) Degenerate in H_0 : $g_n > 1$

Given: $H_0 |\varphi_m^i\rangle = E_m^0 |\varphi_m^i\rangle$, $i \in \{1, 2, \dots q_m\}$

- solutions known exactly for m

$H = H_0 + W$

Question: find the eigenstates + eigenvalues of H

Challenge: no exact solutions

SPT: $W = \lambda \hat{W}$ λ - real #, dimensionless

Goal: $H(\lambda) |\psi_{m,j}(\lambda)\rangle = E_{m,j}(\lambda) |\psi_{m,j}(\lambda)\rangle$

$j \in \{1, \dots q_m\}$

Approach: write $|\psi_{m,j}(\lambda)\rangle$, $E_{m,j}(\lambda)$ as power series in λ

Main results

Non-degenerate: $q_m = 1$

$$E_m \simeq \underbrace{E_m^0}_{\text{0th order}} + \underbrace{\lambda \langle \varphi_m | \hat{W} | \varphi_m\rangle}_{\text{1st order}} + \underbrace{\lambda^2 \sum_{p \neq m} \sum_{i=1}^{q_p} \frac{|\langle \varphi_p^i | \hat{W} | \varphi_m\rangle|^2}{E_m^0 - E_p^0}}_{\text{2nd order}}$$

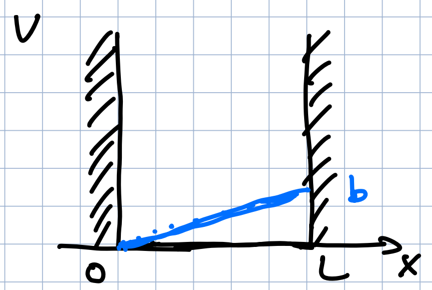
$$\simeq E_m^0 \quad \langle \varphi_m | W | \varphi_m\rangle + \sum_{p \neq m} \sum_{i=1}^{q_p} \frac{|\langle \varphi_p^i | W | \varphi_m\rangle|^2}{E_m^0 - E_p^0}$$

$$|\psi_m\rangle \simeq |\varphi_m\rangle + \lambda \sum_{p \neq m} \sum_{i=1}^{q_p} \frac{\langle \varphi_p^i | \hat{W} | \varphi_m\rangle}{E_m^0 - E_p^0} |\varphi_p^i\rangle$$

$$\simeq |\varphi_m\rangle \quad \sum_{p \neq m} \sum_{i=1}^{q_p} \frac{\langle \varphi_p^i | W | \varphi_m\rangle}{E_m^0 - E_p^0} |\varphi_p^i\rangle$$

$|\psi_m\rangle$ - normalized? - NO

example : non-degenerate perturbation theory



infinite square well

$$\varphi_n(x) = \langle x | \varphi_n \rangle = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

$$n \geq 1$$

$$E_n = n^2 \frac{\hbar^2 \pi^2}{2mL^2} = n^2 \cdot E_1^0 \quad , E_1^0 = \frac{\hbar^2 \pi^2}{2mL^2}$$

Add perturbation:

$$W = b\,\frac{x}{L} \quad , b \ll E_1^0$$

$$\lambda = \frac{b}{E_1^0}$$

$$W = \frac{b}{E_1^0} \cdot E_1^0 \,\frac{x}{L}$$

$$W = \lambda \cdot \hat{W}_1 \quad w/ \quad \lambda \ll 1$$

How does W change the ground state energy and eigenstate?

$$E_1 = E_1^0 + \lambda \langle \varphi_1 | \hat{W} | \varphi_1 \rangle + \lambda^2 \sum_{p \neq n} \sum_{i=1}^{g_p} \frac{|\langle \varphi_p^i | \hat{W} | \varphi_1 \rangle|^2}{E_1^0 - E_p^0}$$

$g_p = 1$ for all states

$$E_1 = E_1^0 + \lambda \langle \varphi_1 | \hat{W} | \varphi_1 \rangle + \lambda^2 \sum_{p=2}^{\infty} \frac{|\langle \varphi_p | \hat{W} | \varphi_1 \rangle|^2}{E_1^0 - E_1^0 \cdot p^2}$$

$$\langle \varphi_p | \hat{W} | \varphi_p \rangle =$$

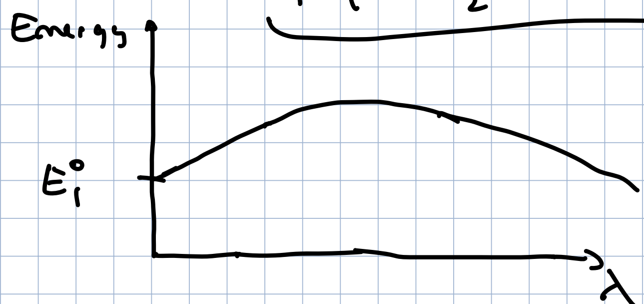
$$= \int_0^L dx\, \frac{2}{L} \sin\left(\frac{\pi x}{L}\right) \cdot \sin\left(\frac{p\pi x}{L}\right) \cdot \frac{x}{L}$$

$$= \begin{cases} \frac{1}{2} & p = 1 \\ -\frac{8p}{\pi^2 (p^2-1)^2} & \text{for } p \geq 2 \text{ even} \\ 0 & \text{for } p \geq 3 \text{ odd} \end{cases}$$

Then: $E_1 = E_1^\circ \left[1 + \lambda \cdot \frac{1}{2} - \lambda^2 \cdot \sum_{\substack{p=2 \\ \text{even}}}^{\infty} \frac{1}{(p^2-1)} \frac{64 p^2}{\pi^4 (p^2-1)^4} \right]$

$$= E_1^\circ \left[1 + \frac{\lambda}{2} - \frac{\lambda^2 \, 64}{\pi^4} \underbrace{\sum_{\substack{p=2 \\ \text{even}}}^{\infty} \frac{p^2}{(p^2-1)^5}}_{\simeq 0.004} \right]$$

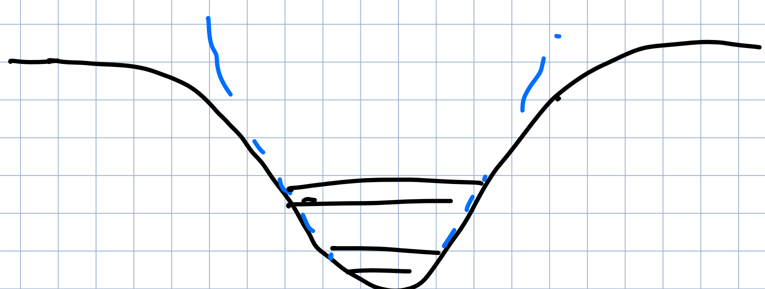
$$= \underbrace{E_1^\circ \left(1 + \frac{\lambda}{2} - 0.011 \lambda^2 \right)} \qquad \text{w/ } \lambda = \frac{b}{E_1}$$



$$\underbrace{|\psi_1\rangle} = |\varphi_1\rangle - \lambda \sum_{\substack{p=2 \\ \text{even}}}^{\infty} \frac{1}{p^2-1} \left(- \frac{8p}{\pi^2 (p^2-1)^2} \right) |\varphi_p\rangle$$

$$= |\varphi_1\rangle + \lambda \sum_{\substack{p=2 \\ \text{even}}}^{\infty} \frac{8}{\pi^2} \frac{p}{(p^2-1)^3} |\varphi_p\rangle =$$

$$= \underbrace{|\varphi_1\rangle} + \lambda \left[\underbrace{0.06} |\varphi_2\rangle + \underbrace{0.001} |\varphi_4\rangle + \underline{0.0001 |\varphi_6\rangle + \dots} \right]$$



Degenerate stationary perturbation theory

CT. , main results

$$\sum_{i'=1}^{g_n} \langle \varphi_n^i | \hat{W} | \varphi_n^{i'} \rangle \langle \varphi_n^{i'} | 0_j \rangle = \epsilon_{j,1} \langle \varphi_n^i | 0_j \rangle$$