

(47)

QM 115B

Lec. 13

Time-Independent Non-Degenerate
Perturbation Theory

$$H = H^0 + \lambda H'$$

we want $H \psi_n = E_n \psi_n$
 we have $H^0 \psi_n^0 = E_n^0 \psi_n^0$

$$\langle \psi_n^0 | \psi_m^0 \rangle = \delta_{mn}$$

$$\psi_n = \psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots$$

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots$$

$$(H^0 + \lambda H')(\psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots) = (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots)(\psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots)$$

$$H^0 \psi_n^0 + \lambda (H^0 \psi_n^1 + H' \psi_n^0) + \lambda^2 (H^0 \psi_n^2 + H' \psi_n^1) + \dots$$

$$= E_n^0 \psi_n^0 + \lambda (E_n^0 \psi_n^1 + E_n^1 \psi_n^0) + \lambda^2 (E_n^0 \psi_n^2 + E_n^1 \psi_n^1 + E_n^2 \psi_n^0) + \dots$$

$$\lambda^0: H^0 \psi_n^0 = E_n^0 \psi_n^0$$

$$\lambda^1: H^0 \psi_n^1 + H' \psi_n^0 = E_n^0 \psi_n^1 + E_n^1 \psi_n^0$$

$$\lambda^2: H^0 \psi_n^2 + H' \psi_n^1 = E_n^0 \psi_n^2 + E_n^1 \psi_n^1 + E_n^2 \psi_n^0$$

$$\text{set } \lambda = 1$$

* first order eq. $H^0 \psi_n' + H' \psi_n^0 = E_n^0 \psi_n' + E_n' \psi_n^0$
inner product

$$\langle \psi_n^0 | H^0 \psi_n' \rangle + \langle \psi_n^0 | H' \psi_n^0 \rangle = E_n^0 \langle \psi_n^0 | \psi_n' \rangle + E_n' \underbrace{\langle \psi_n^0 | \psi_n^0 \rangle}_1$$

$$\langle H^0 \psi_n^0 | \psi_n' \rangle = E_n^0 \langle \psi_n^0 | \psi_n' \rangle$$

$$E_n' = \langle \psi_n^0 | H' | \psi_n^0 \rangle$$

"most import E_2 " in Q.M.

* $(H^0 - E_n^0) \psi_n' = - (H' - E_n') \psi_n^0$

$$\psi_n' = \sum_{m \neq n} c_m^{(n)} \psi_m^0$$

$$\uparrow$$

$$(H^0 - E_n^0) \psi_n^0 = 0$$

$$\sum_{m \neq n} (E_m^0 - E_n^0) c_m^{(n)} \psi_m^0 = - (H' - E_n') \psi_n^0$$

inner prod with ψ_l^0

$$\sum_{m \neq n} (E_m^0 - E_n^0) c_m^{(n)} \langle \psi_l^0 | \psi_m^0 \rangle = - \langle \psi_l^0 | H' \psi_n^0 \rangle + E_n' \langle \psi_l^0 | \psi_n^0 \rangle$$

$$l=n \quad 0 = - \langle \psi_n^0 | H' | \psi_n^0 \rangle + E_n'$$

$$l \neq n: (E_l^0 - E_n^0) c_l^{(n)} = - \langle \psi_l^0 | H' | \psi_n^0 \rangle$$

$$c_m^{(n)} = \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0}$$

$$\text{so } \psi_n' = \sum_{m \neq n} \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0} \psi_m^0$$

$\uparrow$ non-degenerate

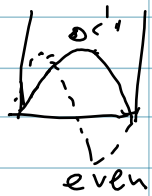
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delta function pert. infinite sq. well
 $0 < x < a$

$$H' = \alpha \delta(x - a/2)$$

$$\psi_n^0 = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

$$\begin{aligned} E_n' &= \langle \psi_n^0 | H' | \psi_n^0 \rangle \\ &= \frac{2}{a} \alpha \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) \delta(x - a/2) dx \\ &= \frac{2\alpha}{a} \sin^2\left(\frac{n\pi}{2}\right) = \frac{2\alpha}{a} \sin^2\left(\frac{n\pi}{2}\right) \\ &= \begin{cases} 0 & n \text{ even} \\ \frac{2\alpha}{a} & n \text{ odd} \end{cases} \end{aligned}$$



$$\psi_1' = \sum_{k \neq 1} \frac{\langle \psi_k^0 | H' | \psi_1^0 \rangle}{E_1^0 - E_k^0} \psi_k^0$$

$$\begin{aligned} \langle \psi_k^0 | H' | \psi_1^0 \rangle &= \frac{2\alpha}{a} \int_0^a \sin\left(\frac{k\pi x}{a}\right) \delta(x - a/2) \sin\left(\frac{\pi x}{a}\right) dx \\ &= \frac{2\alpha}{a} \sin\left(\frac{k\pi a}{2a}\right) \sin\left(\frac{\pi a}{2a}\right) \\ &= \frac{2\alpha}{a} \sin\left(\frac{k\pi}{2}\right) \end{aligned}$$

$$E_1^0 - E_k^0 = \frac{\pi^2 \hbar^2}{2ma^2} (1 - k^2) \quad k = 3, 5, 7, \dots$$

$$\begin{aligned} \psi_1' &= \frac{2\alpha}{a} \frac{2m a^2}{\pi^2 \hbar^2} \left(\frac{-1}{1-9} \psi_3^0 + \frac{1}{1-25} \psi_5^0 - \frac{1}{1-49} \psi_7^0 + \dots \right) \\ &= \frac{4m a \alpha}{\pi^2 \hbar^2} \left(\frac{1}{8} \sin\left(\frac{3\pi x}{a}\right) - \frac{1}{24} \sin\left(\frac{5\pi x}{a}\right) + \frac{1}{48} \sin\left(\frac{7\pi x}{a}\right) - \dots \right) \end{aligned}$$

Second Order

$$H^0 \psi_n^2 + H' \psi_n' = E_n^0 \psi_n^2 + E_n' \psi_n' + E_n^2 \psi_n^0$$

inner prod with ψ_n^0

$$\langle \psi_n^0 | H^0 \psi_n^2 \rangle + \langle \psi_n^0 | H' \psi_n' \rangle =$$

$$\left(= E_n^0 \langle \psi_n^0 | \psi_n^2 \rangle + E_n' \langle \psi_n^0 | \psi_n' \rangle + E_n^2 \langle \psi_n^0 | \psi_n^0 \rangle \right)$$

$$\hookrightarrow \langle \psi_n^0 | H^0 \psi_n^2 \rangle = \langle H^0 \psi_n^0 | \psi_n^2 \rangle = E_n^0 \langle \psi_n^0 | \psi_n^2 \rangle$$

$$E_n^2 = \langle \psi_n^0 | H' | \psi_n' \rangle - E_n' \langle \psi_n^0 | \psi_n' \rangle$$

$$\langle \psi_n^0 | \psi_n' \rangle = \sum_{m \neq n} c_{m,n}^{(n)} \langle \psi_n^0 | \psi_m^0 \rangle = 0$$

$$E_n^2 = \langle \psi_n^0 | H' | \psi_n' \rangle = \sum_{m \neq n} c_m^{(n)} \langle \psi_n^0 | H' | \psi_m^0 \rangle$$

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

$$= \sum_{m \neq n} \frac{|\langle \psi_m^0 | H' | \psi_n^0 \rangle|^2}{E_n^0 - E_m^0}$$