

QM Lecture '18



UNIT TEN: PERTURBATION THEORY

E APPROX. METHODS

MOTTO: A "SMALL" KICK TO THE SYSTEM

NON DEGENERATE PERT. THEORY

- 1) SOLVE \hat{H}_0 SYSTEM "DOMINANT PHYSICS"
- 2) "PERTURB" THE SYSTEM $\hat{H}_0 \rightarrow \hat{H} = \hat{H}_0 + \lambda \hat{H}_1$,
IF λ SMALL, SOLN'S CAN'T BE TOO DIFF.

SPECIALLY

- SUPPOSE WE KNOW $\hat{H}_0 |\psi_n^0\rangle = E_n^0 |\psi_n^0\rangle$
- "0" MEANS "zero" order IN PERT. THY (λ^0)
- IDENTIFY "PERTURBING HAMILTONIAN" H_1 ,
PARAM $\lambda \ll 1$
- PERT. IS THE IDEA TO REP. $\hat{H} |\psi_n\rangle = E_n |\psi_n\rangle$
By $|\psi_n\rangle = \sum_{i=0}^{\infty} \lambda^i |\psi_n^i\rangle$
 $E_n = \sum_{i=0}^{\infty} \lambda^i E_n^i$

GOAL: GIVEN $\hat{H}_0, |\Psi_n^0\rangle, E_n^0$, SOLVE FOR VARIATION
 $|\Psi_n^i\rangle, |E_n^i\rangle$ CORR. $H|\Psi\rangle = E|\Psi\rangle$

PLUG IN $(\hat{H}_0 + \lambda H_1) \sum_{k=0}^{\infty} \lambda^k |\Psi_n^k\rangle = \left(\sum_{k=0}^{\infty} \lambda^k E_n^k \right) \left(\sum_{k=0}^{\infty} \lambda^k |\Psi_n^k\rangle \right)$

SINCE λ ARBITRARY, HOLDS. ORD. BY ORD. IN
 $\lambda \Rightarrow \text{INF } \# \text{ RELATIONS!}$

λ^0 $\hat{H}_0 |\Psi_n^0\rangle = E_n^0 |\Psi_n^0\rangle$ UNPERT. SYS.

λ^1 $\hat{H}_0 |\Psi_n^1\rangle + \hat{H}_1 |\Psi_n^0\rangle = E_n^0 |\Psi_n^1\rangle + E_n^1 |\Psi_n^0\rangle$

λ^2 $\hat{H}_0 |\Psi_n^2\rangle + \hat{H}_1 |\Psi_n^1\rangle = E_n^0 |\Psi_n^2\rangle + E_n^1 |\Psi_n^1\rangle + E_n^2 |\Psi_n^0\rangle$

ISOLATE UNKNOWNNS TO DET THEM

E_n^1 : $\langle \Psi_n^0 | (\lambda^1 \text{ EQN})$

$$\begin{aligned} &\Rightarrow \langle \Psi_n^0 | \hat{H}_0 |\Psi_n^1\rangle + \langle \Psi_n^0 | \hat{H}_1 |\Psi_n^0\rangle = E_n^0 \langle \Psi_n^0 | \Psi_n^1\rangle + E_n^1 \langle \Psi_n^0 | \Psi_n^0\rangle \\ &= E_n^0 \langle \Psi_n^0 | \Psi_n^1\rangle + \langle \Psi_n^0 | \hat{H}_1 |\Psi_n^0\rangle \end{aligned}$$

$$\Rightarrow \boxed{E_n^1 = \langle \Psi_n^0 | \hat{H}_1 |\Psi_n^0\rangle}$$

Q: why does this make sense?

A: just $\langle \hat{H}_1 \rangle$ in the original unperturbed E-st.

$|\Psi_n^1\rangle$: $\langle \Psi_n^0 | \text{ ON } \lambda^1 \text{ EQN } n \neq k$

$$\Rightarrow \langle \Psi_k^0 | \hat{H}_0 |\Psi_n^1\rangle + \langle \Psi_k^0 | \hat{H}_1 |\Psi_n^0\rangle = E_n^0 \langle \Psi_k^0 | \Psi_n^1\rangle + E_n^1 \langle \Psi_k^0 | \Psi_n^0\rangle$$

$$\Rightarrow E_n^0 \langle \Psi_k^0 | \Psi_n^1\rangle + \langle \Psi_k^0 | \hat{H}_1 |\Psi_n^0\rangle = E_n^0 \langle \Psi_k^0 | \Psi_n^1\rangle$$

$$\Rightarrow \langle \Psi_n^0 | \Psi_n' \rangle = \frac{\langle \Psi_n^0 | \hat{H}_1 | \Psi_n^0 \rangle}{E_n^0 - E_k^0} \quad *_{\text{INT}}$$

Now $|\Psi_n'\rangle = \sum_{k=0}^{\infty} |\Psi_k^0\rangle \langle \Psi_k^0 | \Psi_n' \rangle = |\Psi_n^0\rangle \langle \Psi_n^0 | \Psi_n' \rangle + \sum_{k \neq n} |\Psi_k^0\rangle \langle \Psi_k^0 | \Psi_n' \rangle$

?
*_{INT}

$$\langle \Psi_n^0 | \Psi_n' \rangle$$

1 BC ORIG E-ST.

NOTE: $1 - \langle \Psi_n | \Psi_n \rangle = \underbrace{\langle \Psi_n^0 | \Psi_n^0 \rangle}_{=0 \text{ REQ.}} + \lambda \{ \langle \Psi_n^0 | \Psi_n' \rangle + \langle \Psi_n' | \Psi_n^0 \rangle \} + O(\lambda^2)$

$$\langle \Psi_n^0 | \Psi_n' \rangle = ia, a \in \mathbb{R}$$

THEN $|\Psi_n\rangle = |\Psi_n^0\rangle + \lambda |\Psi_n'\rangle$

$$= |\Psi_n^0\rangle + \lambda \{ |\Psi_n^0\rangle \langle \Psi_n^0 | \Psi_n' \rangle + \sum_{k \neq n} |\Psi_k^0\rangle \langle \Psi_k^0 | \Psi_n' \rangle \} + O(\lambda^2)$$

$$= |\Psi_n^0\rangle + \lambda ia |\Psi_n^0\rangle + \text{SAME} = (1 + \lambda ia) |\Psi_n^0\rangle + \text{SAME}$$

$$= e^{ia\lambda} |\Psi_n^0\rangle + \text{SAME}$$

↑ TRUE TO + O(λ)

$$= e^{ia\lambda} \left(|\Psi_n^0\rangle + (1-ia\lambda) \lambda \sum_{k \neq n} |\Psi_k^0\rangle \langle \Psi_k^0 | \Psi_n' \rangle \right) + O(\lambda^2)$$

$$= e^{ia\lambda} \left(|\Psi_n^0\rangle + \lambda \sum_{k \neq n} |\Psi_k^0\rangle \langle \Psi_k^0 | \Psi_n' \rangle \right) + O(\lambda^2)$$

IRREL

EFT. SET $a=0 \Rightarrow \langle \Psi_n^0 | \Psi_n' \rangle = 0$ *

$\therefore |\Psi_n\rangle = |\Psi_n^0\rangle + \lambda \sum_{k \neq n} |\Psi_k^0\rangle \frac{\langle \Psi_k^0 | \hat{H}_1 | \Psi_k^0 \rangle}{E_k^0 - E_n^0}$

FROM ABOVE

WORDS TO $0(\lambda)$, $|\Psi_n^0\rangle$ IS $|\Psi_n\rangle$

PLUS WEIGHTED SUM OVER ALL $|\Psi_{k \neq n}^0\rangle$

$$\underline{E_n^2} \quad \lambda^2 \text{ TERM: } \hat{H}_0 |\Psi_n^2\rangle + \hat{H}_1 |\Psi_n^1\rangle = E_n^0 |\Psi_n^2\rangle + E_n^1 |\Psi_n^1\rangle + E_n^2 |\Psi_n^0\rangle$$

Now $\langle \Psi_n^0 |$ IT

$$\begin{aligned} \langle \Psi_n^0 | \hat{H}_0 | \Psi_n^2 \rangle + \langle \Psi_n^0 | \hat{H}_1 | \Psi_n^1 \rangle &= E_n^0 \langle \Psi_n^0 | \Psi_n^2 \rangle + E_n^1 \langle \Psi_n^0 | \Psi_n^1 \rangle \\ &\quad + E_n^2 \langle \Psi_n^0 | \Psi_n^0 \rangle \end{aligned}$$

*i α_1 but
 $\alpha=0$*

$$\begin{aligned} \Rightarrow E_n^2 &= \langle \Psi_n^0 | \hat{H}_1 | \Psi_n^1 \rangle \\ &= \langle \Psi_n^0 | \hat{H}_1 | \Psi_n^0 \rangle \underbrace{\langle \Psi_n^0 | \Psi_n^1 \rangle}_{\text{cancel}} + \sum_{k \neq n} \langle \Psi_k^0 | \Psi_n^1 \rangle \end{aligned}$$
$$= \sum_{k \neq n} \underbrace{\langle \Psi_k^0 | \hat{H}_1 | \Psi_k^0 \rangle}_{\langle \Psi_k^0 | \hat{H}_1 | \Psi_k^0 \rangle} \langle \Psi_k^0 | \Psi_n^1 \rangle$$
$$= \frac{\langle \Psi_k^0 | \hat{H}_1 | \Psi_k^0 \rangle}{E_n^0 - E_k^0} \quad (\text{SAW})$$

$$\Rightarrow \boxed{E_n^2 = \sum_{k \neq n} \frac{|\langle \Psi_k^0 | \hat{H}_1 | \Psi_k^0 \rangle|^2}{E_n^0 - E_k^0}}$$

EX: S.H.O. IN \vec{E} -FIELD

$$\hat{H}_0 = \frac{\vec{P}_x^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 \quad \hat{H}_1 = -g |\vec{E}| \hat{x} \text{ since } (\vec{F} = g|\vec{E}|\hat{i})$$

FIRST E-CORR.

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

$$\bar{E}_n^1 = \langle n | \hat{H}_1 | n \rangle = -g |\vec{E}| \langle n | \hat{x} | n \rangle = -g |\vec{E}| \cancel{\langle n | \hat{x} | n \rangle} = 0$$

comp pres.

SECOND E-CORR

$$E_n^2 = \sum_{k \neq n} \frac{|\langle k | H_1 | n \rangle|^2}{E_n^0 - E_k^0}$$

$$\begin{aligned} \langle k | H_1 | n \rangle &= -g |\vec{E}| \langle k | \hat{x} | n \rangle = -g \bar{E} \sqrt{\frac{\hbar}{2m\omega}} (\langle k | (a + a^\dagger) | n \rangle) \\ &= -g \bar{E} \sqrt{\frac{\hbar}{2m\omega}} \left\{ \sqrt{n+1} \langle k | n+1 \rangle + \sqrt{n} \langle k | n-1 \rangle \right\} \end{aligned}$$

ONLY to FOR $k = n \pm 1$

$$\Rightarrow E_n^2 = \frac{g^2 |\vec{E}|^2 \hbar}{2m\omega} \left\{ \frac{n+1}{-\hbar\omega} + \frac{n}{\hbar\omega} \right\}$$

$$\Rightarrow \boxed{E_n^2 = -\frac{g^2 |\vec{E}|^2}{2m\omega^2}}$$

NOTE: INDEP OF N! LEADING SHIFT IS
OF ALL E-LEV BY SAME AMT.

DO HIGHER CORRS! (guesses? why? why not?)

NO HIGHER CORR!

PROOF

$$\begin{aligned} H &= \frac{p_x^2}{2m} + \frac{1}{2} m \omega^2 x^2 - g |\vec{E}| x \\ &= \frac{p_x^2}{2m} + \frac{1}{2} m \cdot \omega \left(\hat{x} - \frac{g |\vec{E}|}{m \omega^2} \right)^2 - \frac{g^2 |\vec{E}|^2}{2m \omega^2} \\ &=: \frac{p_x^2}{2m} + \frac{1}{2} m \omega \hat{x}^2 - \frac{g^2 |\vec{E}|^2}{2m \omega^2} \\ &=: \tilde{H}_{S.H.O.} - \frac{g^2 |\vec{E}|^2}{2m \omega^2} \\ \Rightarrow E_n &= \left(n + \frac{1}{2} \right) \hbar \omega - \frac{g^2 |\vec{E}|^2}{2m \omega^2} = \left(n + \frac{1}{2} \right) \hbar \omega + E_n^2 \end{aligned}$$

SO E_n^2 IS ONLY ENERGY CORR.

Q: WHAT'S THE FLAW w/ ALL THIS?

A: $\frac{1}{E_n^0 - E_k^0}$ CORR. $\Rightarrow \frac{1}{0} !?$

DEGENERATE PERTURBATION THEORY

DEGENERACY: MULTIPLE H_0 E-STATES @ SAME E

- * FIX EN. LEV. E_n^0
- * SUPPOSE \exists g_n STATES \in PERT TO g_n STATES $| \Psi_{n,i} \rangle$
- * HAVE DEGENERATE SYSTEM

$$| \Psi_{n,i} \rangle \quad i = 1, \dots, g_n$$

$$| \Psi_n^0 \rangle \quad c = 1, \dots, g_n$$

\hat{c} suppose $| \Psi_{n,i} \rangle = \underbrace{\sum_{j=1}^{g_n} c_{ij} | \Psi_n^0 \rangle}_{\text{EN. E-ST.}} + \lambda \underbrace{| \Psi_n' \rangle}_{\text{PERT. CORR.}}$

$$(H_0 + \lambda H_1) | \Psi_{n,i} \rangle = H_0 | \Psi_{n,i} \rangle + \lambda H_1 \sum_{j=1}^{g_n} c_{ij} | \Psi_n^0 \rangle + O(\lambda)$$

$$= \sum_{ij} c_{ij} E_n^0 | \Psi_n^0 \rangle + \lambda \left(H_0 | \Psi_n' \rangle + \sum_{j=1}^{g_n} c_{ij} H_1 | \Psi_n^0 \rangle \right)$$

$$\boxed{= E_n^{(0)} | \Psi_n^{(0)} \rangle + E_n^{(0)} \sum_{n=1}^{g_n} c_{ij} | \Psi_n^{(0)} \rangle} \xrightarrow{\langle \Psi_{n,i} |} \sum_{j=1}^{g_n} \langle \Psi_{n,i} | \hat{H}_1 | \Psi_n^0 \rangle c_{ij} = \sum_{j=1}^{g_n} c_{ij} E_n^0 \langle \Psi_{n,i} | \Psi_n^0 \rangle$$

* SUPPOSE IN n^{th} DEGEN. SEC. $\langle \Psi_{n,i} | \Psi_{n,j}^0 \rangle = \delta_{ij}$

$$\Rightarrow \boxed{\sum_{j=1}^{g_n} c_{ij} [(\hat{H}_1)_{ij} - E_n^0 \delta_{ij}] = 0} \Rightarrow \hat{H}_1 \vec{c} = E_n^0 \vec{c}$$

* SOLVE EIGENSYSTEM TO GET C'S, E'S, $\therefore | \Psi_{n,i} \rangle$ 'S

* SUMMARY DIAG. PERT. \hat{H}_1 WRT. UNPERTURBED STATES!

* g_n DIST. E'S \Rightarrow NON-DEGEN @ $O(\lambda)$

EXAMPLE: STARK EFFECT IN HYDROGEN

* UNIFORM \vec{E}

$$* \text{ PERT BY } \hat{H}_1 = -\frac{\gamma}{m} \cdot \vec{E} = e \hat{r} \cdot \vec{E} = e |\vec{E}| \hat{z}$$

$$\therefore \hat{H}_0 = \frac{\hat{p}^2}{2m} - \frac{e^2}{|\vec{r}|}$$

$$|\Psi_h^0\rangle = \underbrace{|n, l, m\rangle}_{\substack{\text{DEGENERACY} \\ \text{LABELS}}}$$

DEGENERACY
LABELS

* GROUND STATE $n=1 \quad l=0 \quad \text{NON DEGEN} \quad E_1^1=0 \quad E_1^2 \neq 0$

* $n=2$ 4 DEGEN STATES $\{ |200\rangle, |211\rangle, |210\rangle, |21,-1\rangle \}$

* DIAG \hat{H}_1 IN UNPERT. BASIS. (would think ^{need} 10 elements. not so!)

① SIMP. Y_{lm} PARITY $(-1)^l$. \hat{z} ODD IN POS SPACE

$$\Rightarrow \langle l, m | \hat{z} | l', m' \rangle \neq 0 \quad \text{IFF} \quad l \neq l'$$

∴ COMP. ONLY $l=1, l'=0$ COMBS

② $[L_z, z] = 0 \Rightarrow [\hat{H}_1, L_z] = 0 \Rightarrow \hat{H}_1 \text{ CONSERVES } m$

$$\Rightarrow \text{ONLY } \langle 200 | \hat{H}_1 | 210 \rangle = e |\vec{E}| \langle 200 | \hat{z} | 210 \rangle \neq 0$$

$$= -3e |\vec{E}| a_0$$

↑ (just doing an integral)

$$\Rightarrow \begin{vmatrix} -E_2^1 & -3e |\vec{E}| a_0 & & \\ -E_2^1 & & & \\ -3e |\vec{E}| a_0 & -E_2^1 & & \\ & & -E_2^1 & \end{vmatrix} = 0 = (E_2^1)^4 - (E_2^1)^2 3e |\vec{E}| a_0 = 0$$

$E_2^1 \in \{0, 0, \pm \underbrace{3e |\vec{E}| a_0}_{\Delta}\}$

— 1
— 2 STATES
— 1

$-E_2^1 = 0: \quad 2 \text{ STATES, NEED HIGHER ORDER}$

$-E_2^1 = -\Delta: \quad E = E^0 - 3e |\vec{E}| a_0 \quad \frac{1}{\sqrt{2}} \{ |200\rangle + |210\rangle \}$

$-E_2^1 = \Delta \quad E = E^0 + 3e |\vec{E}| a_0 \quad \frac{1}{\sqrt{2}} \{ |200\rangle - |210\rangle \}$