QM Lecture 18

UNIT TEN: PERTURBATION THEORY & 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 $\hat{H}_0 \longrightarrow \hat{H} = \hat{H}_0 + \lambda \hat{H}_1$

   IF λ SMALL, SOLN'S CAN'T BE TOO DIFF.

SPECIFICALLY

- SUPPOSE WE KNOW $\hat{H}_0 |\varphi_n^0\rangle = E_n^0 |\varphi_n^0\rangle$
- "0" MEANS "zeroth order" IN PERT. THY (λ^0)
- IDENTIFY "PERTUBING HAMILTONIAN" H_1

  & PARAM $\lambda \ll 1$
- PERT. IS THE IDEA TO REP. $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$

  By $|\psi_n\rangle = \sum_{i=0}^{\infty} \lambda^i |\varphi_n^i\rangle$

  $E_n = \sum_{i=0}^{\infty} \lambda^i E_n^i$

GOAL: GIVEN $\hat{H}_0$, $|\varphi_n^0\rangle$, E_n^0, SOLVE FOR LEADING $|\varphi_n^i\rangle$, $|E_n^i\rangle$ CORR.

$H|\varphi\rangle = E|\varphi\rangle$

PLUG IN $$(H_0 + \lambda H_1)\sum_{k=0}^{\infty} \lambda^k |\varphi_n^k\rangle = \left(\sum_{k=0}^{\infty} \lambda^k E_n^k\right)\left(\sum_{k=0}^{\infty} \lambda^k |\varphi_n^k\rangle\right)$$

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

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

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

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

ISOLATE UNKNOWNS TO DET THEM

E_n^1: $\langle\varphi_n^0|$ (λ^1 EQN)

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

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

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

Q: why does this make sense?

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

$|\varphi_n^1\rangle$: $\langle\varphi_k^0|$ ON λ^1 EQN $\quad n \neq k$

$$\Rightarrow \langle\varphi_k^0|\hat{H}_0|\varphi_n^1\rangle + \langle\varphi_k^0|\hat{H}_1|\varphi_n^0\rangle = E_n^0\langle\varphi_k^0|\varphi_n^1\rangle + E_n^1\cancelto{0}{\langle\varphi_k^0|\varphi_n^0\rangle}$$

$$\Rightarrow E_k^0\langle\varphi_k^0|\varphi_n^1\rangle + \langle\varphi_k^0|\hat{H}_1|\varphi_n^0\rangle = E_n^0\langle\varphi_k^0|\varphi_n^1\rangle$$

$$\Rightarrow \langle \varphi_k^0 | \varphi_n^1 \rangle = \frac{\langle \varphi_k^0 | \hat{H}_1 | \varphi_n^0 \rangle}{E_n^0 - E_k^0} \qquad *_{INT}$$

NOW $$|\varphi_n^1\rangle = \sum_{k=0}^{\infty} |\varphi_k^0\rangle \langle \varphi_k^0 | \varphi_n^1 \rangle = |\varphi_n^0\rangle \overbrace{\langle \varphi_n^0 | \varphi_n^1 \rangle}^{?} + \sum_{k \neq n} |\varphi_k^0\rangle \underbrace{\langle \varphi_k^0 | \varphi_n^1 \rangle}_{*_{INT}}$$

$\langle \varphi_n^0 | \varphi_n^1 \rangle$

NOTE: $$1 = \langle \psi_n | \psi_n \rangle = \overbrace{\langle \varphi_n^0 | \varphi_n^0 \rangle}^{1 \text{ BC ORIG E-ST.}} + \lambda \underbrace{\{\langle \varphi_n^0 | \varphi_n^1 \rangle + \langle \varphi_n^1 | \varphi_n^0 \rangle\}}_{=0 \text{ REQ.}} + O(\lambda^2)$$

$$\langle \varphi_n^0 | \varphi_n^1 \rangle = ia, \quad a \in \mathbb{R}$$

THEN $$|\psi_n\rangle = |\varphi_n^0\rangle + \lambda |\varphi_n^1\rangle$$

$$= |\varphi_n^0\rangle + \lambda \{ |\varphi_n^0\rangle \langle \varphi_n^0 | \varphi_n^1 \rangle + \sum_{k \neq n} |\varphi_k^0\rangle \langle \varphi_k^0 | \varphi_n^1 \rangle \} + O(\lambda^2)$$

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

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

TRUE TO $+ O(\lambda)$

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

$$= \cancel{e^{ia\lambda}} \left(|\varphi_n^0\rangle + \lambda \sum_{k \neq n} |\varphi_k^0\rangle \langle \varphi_k^0 | \varphi_n^1 \rangle \right) + O(\lambda^2)$$

IRREL

EFF. SET $a = 0 \Rightarrow \langle \varphi_n^0 | \varphi_n^1 \rangle = 0 \quad **$

FROM ABOVE

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

$\underline{\text{WORDS}}$ TO $O(\lambda)$, $|\psi_n^0\rangle$ IS $|\varphi_n^0\rangle$
PLUS WEIGHTED SUM OVER ALL $|\varphi_{k\neq n}^0\rangle$

$\underline{E_n^2}$ λ^2 TERM: $\hat{H}_0|\varphi_n^2\rangle + \hat{H}_1|\varphi_n^1\rangle = E_n^0|\varphi_n^2\rangle + E_n^1|\varphi_n^1\rangle + E_n^2|\varphi_n^0\rangle$

NOW $\langle\varphi_n^0|$ IT

ie, but $a=0$

$$\langle\varphi_n^0|\hat{H}_0|\varphi_n^2\rangle + \langle\varphi_n^0|\hat{H}_1|\varphi_n^1\rangle = E_n^0\langle\varphi_n^0|\varphi_n^2\rangle + E_n^1\underbrace{\langle\varphi_n^0|\varphi_n^1\rangle}_{} + E_n^2\underbrace{\langle\varphi_n^0|\varphi_n^0\rangle}_{1}$$

$$= E_n^0\langle\varphi_n^0|\varphi_n^2\rangle + \text{''}$$

$$\Rightarrow E_n^2 = \langle\varphi_n^0|\hat{H}_1|\varphi_n^1\rangle$$

$$= \langle\varphi_n^0|\hat{H}_1\left\{|\varphi_n^0\rangle\cancelto{0}{\langle\varphi_n^0|\varphi_n^1\rangle} + \sum_{k\neq n}|\varphi_k^0\rangle\langle\varphi_k^0|\varphi_n^1\rangle\right\}$$

$$= \sum_{k\neq n}\langle\varphi_n^0|H_1|\varphi_k^0\rangle\underbrace{\langle\varphi_k^0|\varphi_n^1\rangle}_{= \frac{\langle\varphi_k^0|\hat{H}_1|\varphi_n^0\rangle}{E_n^0 - E_k^0}}$$

(SAW)

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

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

$$\hat{H}_0 = \frac{P_x^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 \qquad \hat{H}_1 = -q|\vec{E}|\,\hat{x} \quad \text{since } \left(\vec{F} = q|\vec{E}|\,\hat{i}\right)$$

FIRST E-CORR.

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

comp prev.

$$E_n^1 = \langle n|\hat{H}_1|n\rangle = -q|\vec{E}|\langle n|\hat{x}|n\rangle = -q|\vec{E}|\cancelto{0}{\langle x\rangle} = 0$$

SECOND E-CORR

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

$$\langle k|H_1|n\rangle = -q|\vec{E}|\langle k|x|n\rangle = -qE\sqrt{\frac{\hbar}{2m\omega}}\left(\langle k|(a+a^\dagger)|n\rangle\right)$$

$$= -qE\sqrt{\frac{\hbar}{2m\omega}}\left\{\sqrt{n+1}\,\langle k|n+1\rangle + \sqrt{n}\,\langle k|n-1\rangle\right\}$$

ONLY $\neq 0$ FOR $k = n \pm 1$

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

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

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

DO $\exists$ HIGHER CORRS!? (guesses? why? why not?)

NO HIGHER CORR!

PROOF

$$H = \frac{p_x^2}{2m} + \frac{1}{2} m\omega^2 x^2 - q|\vec{E}|x$$

$$= \frac{p_x^2}{2m} + \frac{1}{2} m\omega \left(\hat{x} - \frac{q|\vec{E}|}{m\omega^2}\right)^2 - \frac{q^2 |E|^2}{2m\omega^2}$$

$$=: \frac{p_x^2}{2m} + \frac{1}{2} m\omega \hat{\tilde{x}}^2 - \frac{q^2|E|^2}{2m\omega^2}$$

$$=: \tilde{H}_{S.H.O.} - \frac{q^2|E|^2}{2m\omega^2}$$

$$\Longrightarrow \quad E_n = \left(n+\tfrac{1}{2}\right)\hbar\omega - \frac{q^2|\vec{E}|^2}{2m\omega^2} = \left(n+\tfrac{1}{2}\right)\hbar\omega + E_n^2$$

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. $\Longrightarrow \frac{1}{0}$!?

DEGENERATE PERTURBATION THEORY

DEGENERACY: MULTIPLE H_0 E-STATES @ SAME E

* FIX EN. LEV. E_n^0
* SUPPOSE $\exists$ g_n STATES & PERT TO g_n STATES $|\psi_n\rangle$
* HAVE DEGENERATE SYSTEM

$$|\psi_{n,i}\rangle \qquad i=1,\dots,g_n$$
$$|\varphi^0_{n,i}\rangle \qquad i=1,\dots,g_n$$

& SUPPOSE
$$|\psi_{n,i}\rangle = \underbrace{\sum_{j=1}^{g_n} c_{ij}\,|\varphi^0_{n,j}\rangle}_{\text{EN. E-ST., SAME } E} + \lambda \underbrace{|\varphi_n'\rangle}_{\text{PERT. CORR.}} + \dots$$

$$(H_0+\lambda H_1)|\psi_{n,i}\rangle =$$

$$H_0|\psi_n\rangle + \lambda H_1 \sum_{j=1}^{g_n} c_{ij}|\varphi^0_{n,j}\rangle + O(\lambda^2) = \sum c_{ij} E_n^0 |\varphi^0_{n,j}\rangle + \lambda\left(\underbrace{H_0|\varphi_n'\rangle + \sum_{j=1} c_{ij} H_1|\varphi^0_{n,j}\rangle}\right)$$

$$= E_n^{(0)}|\varphi_n^{(1)}\rangle + \lambda E_n^{(1)} \sum_{n=1}^{g_n} c_{ij}|\varphi^{(0)}_{n,j}\rangle \xrightarrow{\langle\varphi_{n,i}^0|} \sum_{j=1}^{g_n} \langle\varphi^0_{n,i}|\hat{H}_1|\varphi^0_{n,j}\rangle c_{ij} = \sum_{j=1}^{g_n} c_{ij} E_n^1 \langle\varphi^0_{n,i}|\varphi^0_{n,j}\rangle$$

terms w/ H_0, E_n^0 cancel

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

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

* SOLVE EIGENSYSTEM TO GET c's, $E^{(1)}$'s, & $\therefore$ $|\psi_{n,i}\rangle$'s
* SUMMARY DIAG. PERT. $\hat{H}_1$ WRT. UNPERTURBED STATES!
* g_n DIST. E^1's $\Rightarrow$ NON-DEGEN @ $O(\lambda)$

EXAMPLE: STARK EFFECT IN HYDROGEN

* UNIFORM $\vec{E}$
* PERT BY $\hat{H}_1 = -\hat{\vec{\mu}} \cdot \vec{E} = e\hat{\vec{r}} \cdot \vec{E} = e|\vec{E}|\hat{z}$

$$\therefore \quad \hat{H}_0 = \frac{\hat{p}^2}{2m} - \frac{e^2}{|\vec{r}|} \qquad |\varphi_n^0\rangle = |n, \underbrace{l, m}_{\text{DEGENERACY LABELS}}\rangle$$

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

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

* 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

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

$$= \langle l, m|\pi^{\dagger}\pi z \pi^{\dagger}\pi|l', m'\rangle$$

$$= (-1)^{l+l'+1} \cdot \text{same}$$

$\therefore$ COMP. ONLY $l=1$, $l'=0$ COMBS

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

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

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

(just doing an integral)

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

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

— 1
— 2 STATES
— 1

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