TIME - INDEPENDENT PERTURBATION THEORY

⇒ NONDEGENERATE PERTURBATION THEORY

• **INTRO**

↳ SUPPOSE WE HAVE SOLVED

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

(UNPERTURBED PROBLEM)

↳ SUPPOSE WE WANT TO SOLVE SCHRODINGER EQ. IN PRESENCE OF SMALL PERTURBATION (e.g. H ATOM IN WEAK APPLIED MAGNETIC FIELD)

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

↑ SMALL PERTURBATION

(λ PARAMETER TO DENOTE ORDER OF PERTURBATION WILL BE TAKEN → 1 IN END)

$$H|\psi_n\rangle = E_n|\psi_n\rangle$$

CAN WE FIND APPROXIMATE SOLUTIONS FOR $|\psi_n\rangle$ & E_n ?

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

$$E_n = \underset{\substack{\Uparrow \\ \text{KNOWN}}}{E_n^0} + \lambda \underset{\substack{\Uparrow \\ \text{1-ORDER} \\ \text{CORRECTION}}}{E_n^1} + \lambda^2 \underset{\substack{\Uparrow \\ \text{2-ORDER} \\ \text{CORRECTION}}}{E_n^2} + \dots$$

$\downarrow$ $H|\psi_n\rangle = E_n|\psi_n\rangle$

$$(H^0 + \lambda H^1)\left(|\psi_n^0\rangle + \lambda|\psi_n^1\rangle + \lambda^2|\psi_n^2\rangle + \dots\right)$$

$$= \left(E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots\right)\left(|\psi_n^0\rangle + \lambda|\psi_n^1\rangle + \lambda^2|\psi_n^2\rangle + \dots\right)$$

$\downarrow$ EXPANSION IN λ

$$H^0|\psi_n^0\rangle + \lambda\left(H^1|\psi_n^0\rangle + H^0|\psi_n^1\rangle\right) + \lambda^2\left(H^1|\psi_n^1\rangle + H^0|\psi_n^2\rangle\right) + \dots$$

$$= E_n^0|\psi_n^0\rangle + \lambda\left(E_n^1|\psi_n^0\rangle + E_n^0|\psi_n^1\rangle\right) + \lambda^2\left(E_n^0|\psi_n^2\rangle + E_n^1|\psi_n^1\rangle + E_n^2|\psi_n^0\rangle\right) + \dots$$

$\downarrow$ IDENTIFY TERMS IN λ-EXPANSION

↳ TO LOWEST ORDER λ^0 :

$$H^0|\psi_n^0\rangle = E_n^0|\psi_n^0\rangle$$ ORIGINAL , UNPERTURBED PROBLEM WHICH WE HAVE SOLVED

↳ TO FIRST ORDER λ^1

$$H^1|\psi_n^0\rangle + H^0|\psi_n^1\rangle = E_n^1|\psi_n^0\rangle + E_n^0|\psi_n^1\rangle$$

↳ TO SECOND ORDER λ^2 :

$$H^1|\psi_n^1\rangle + H^0|\psi_n^2\rangle = E_n^0|\psi_n^2\rangle + E_n^1|\psi_n^1\rangle + E_n^2|\psi_n^0\rangle$$

- **FIRST - ORDER PERTURBATION THEORY**

↳ $$H^1|\psi_n^0\rangle + H^0|\psi_n^1\rangle = E_n^1|\psi_n^0\rangle + E_n^0|\psi_n^1\rangle$$

↓ TAKE INNER PRODUCT WITH $\langle\psi_n^0|$

$$\langle\psi_n^0|H^1|\psi_n^0\rangle + \langle\psi_n^0|H^0|\psi_n^1\rangle$$

$$= E_n^1\langle\psi_n^0|\psi_n^0\rangle + E_n^0\langle\psi_n^0|\psi_n^1\rangle$$

↓ $$\langle\psi_n^0|H^0 = \langle\psi_n^0|E_n^0$$

$$\langle\psi_n^0|\psi_n^0\rangle = 1$$

$$\langle \psi_n^0 | H^1 | \psi_n^0 \rangle + \cancel{E_n^0 \langle \psi_n^0 | \psi_n^1 \rangle}$$

$$= E_n^1 + \cancel{E_n^0 \langle \psi_n^0 | \psi_n^1 \rangle}$$

$$\Downarrow$$

$$\boxed{E_n^1 = \langle \psi_n^0 | H^1 | \psi_n^0 \rangle}$$

NOTE: WE USE THIS WHEN CALCULATING THE CORRECTION DUE TO COULOMB REPULSION BETWEEN $2e^-$ IN He ATOM:

$$H^1 = \frac{e^2}{4\pi \varepsilon_0 |\bar{r}_1 - \bar{r}_2|}$$

↳ $|\psi_n^1\rangle$ (FIRST ORDER CORRECTION TO WAVE FUNCTION)

$$(H^0 - E_n^0)|\psi_n^1\rangle = (E_n^1 - H^1)|\psi_n^0\rangle$$

$|\psi_m^0\rangle$ FORMS COMPLETE SET

$$\boxed{|\psi_n^1\rangle = \sum_{m \neq n} c_m^{(n)} |\psi_m^0\rangle}$$

NOTE: TERM $|\psi_n^0\rangle$ DOES NOT CONTRIBUTE AS $(H^0 - E_n^0)|\psi_n^0\rangle = 0$

NOTE $\quad \underset{\sim\sim\sim}{C_n^{(n)} = 0}$

$$C_n^{(n)} \equiv \langle \psi_n^0 | \psi_n^1 \rangle$$

NORMALIZATION $\quad \langle \psi_n^0 | \psi_n^0 \rangle = 1$

$$\langle \psi_n | \psi_n \rangle = 1$$

WITH $\quad |\psi_n\rangle = |\psi_n^0\rangle + \lambda |\psi_n^1\rangle$

TO ORDER λ

$$\langle \psi_n^0 | \psi_n^1 \rangle + \langle \psi_n^1 | \psi_n^0 \rangle = 0$$

$$\mathrm{Re}\, C_n^{(n)} = 0$$

WE CAN MAKE A CHANGE OF PHASE

$$|\psi_n\rangle \rightarrow e^{i\lambda\alpha} |\psi_n\rangle$$

AND CHOOSE α SUCH THAT $\mathrm{Im}\, C_n^{(n)} = 0$

$$\therefore \quad \underline{\underline{C_n^{(n)} = 0}}$$

$$\sum_{m \neq n} (H^0 - E_n^0)\, c_m^{(n)} |\psi_m^0\rangle = (E_n^1 - H^1)|\psi_n^0\rangle$$

$\downarrow$ $|\psi_m^0\rangle$ ARE EIGENSTATES OF H^0

$$\sum_{m \neq n} c_m^{(n)} (E_m^0 - E_n^0)|\psi_m^0\rangle = (E_n^1 - H^1)|\psi_n^0\rangle$$

$\downarrow$ $\langle \psi_\ell^0|$

$$\sum_{m \neq n} c_m^{(n)} (E_m^0 - E_n^0) \langle \psi_\ell^0 | \psi_m^0 \rangle$$

$$= E_n^1 \langle \psi_\ell^0 | \psi_n^0 \rangle - \langle \psi_\ell^0 | H^1 | \psi_n^0 \rangle$$

CASE $\ell = n$ $\quad \langle \psi_\ell^0 | \psi_m^0 \rangle = 0$

$$\rightsquigarrow E_n^1 = \langle \psi_n^0 | H^1 | \psi_n^0 \rangle$$

OK! WE DERIVED THIS BEFORE

CASE $\ell \neq n$ $\quad \langle \psi_\ell^0 | \psi_m^0 \rangle = \delta_{\ell m}$

$$c_\ell^{(n)} \left(E_\ell^\circ - E_n^\circ \right) = - \langle \psi_\ell^\circ | H' | \psi_n^\circ \rangle$$

$$c_\ell^{(n)} = \frac{\langle \psi_\ell^\circ | H' | \psi_n^\circ \rangle}{E_n^\circ - E_\ell^\circ}$$

$$\therefore \boxed{ |\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^\circ | H' | \psi_n^\circ \rangle}{E_n^\circ - E_m^\circ} |\psi_m^\circ\rangle }$$

ONLY APPLIES WHEN UNPERTURBED SPECTRUM is NON DEGENERATE (i.e. NO 2 ENERGIES E_m° ARE SAME)

- SECOND ORDER PERTURBATION THEORY

$$H'|\psi_n^1\rangle + H^\circ|\psi_n^2\rangle = E_n^\circ|\psi_n^2\rangle + E_n^1|\psi_n^1\rangle + E_n^2|\psi_n^\circ\rangle$$

$$\downarrow \quad \langle \psi_n^\circ |$$

$$\langle \psi_n^\circ | H' | \psi_n^1 \rangle + \cancel{\langle \psi_n^\circ | H^\circ | \psi_n^2 \rangle}$$

$$= \cancel{E_n^\circ \langle \psi_n^\circ | \psi_n^2 \rangle} + E_n^1 \langle \psi_n^\circ | \psi_n^1 \rangle + E_n^2$$

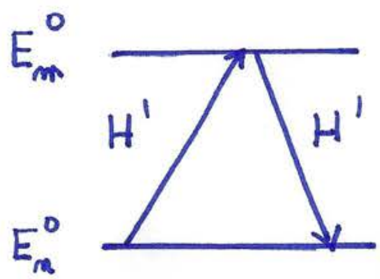
$$\downarrow \quad \langle \psi_n^\circ | H^\circ = \langle \psi_n^\circ | E_n^\circ$$

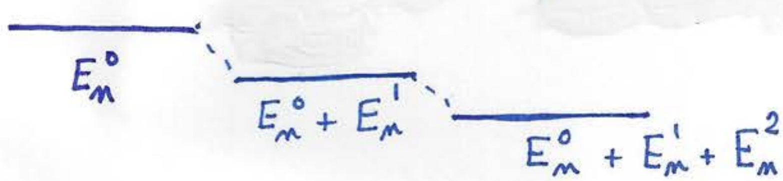
6.7

$$E_n^{(2)} = \langle \psi_n^0 | H' | \psi_n^1 \rangle - E_n^1 \underbrace{\langle \psi_n^0 | \psi_n^1 \rangle}_{0}$$

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

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





⇒ DEGENERATE PERTURBATION THEORY

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

$\downarrow$

2 ENERGIES $E_m^0 = E_n^0$ (FOR $m \neq n$)

$\downarrow$

E_n^2 BLOWS UP → DERIVATION DOES NOT APPLY

- **2 - FOLD DEGENERACY**

↳ $E_a^0 = E_b^0 = E^0$

$$\left.\begin{aligned} H^0 |\psi_a^0\rangle &= E^0 |\psi_a^0\rangle \\ H^0 |\psi_b^0\rangle &= E^0 |\psi_b^0\rangle \end{aligned}\right\}$$

ANY LIN. COMB. $\alpha |\psi_a^0\rangle + \beta |\psi_b^0\rangle$ STILL SOLUTION OF H^0

$\langle \psi_a^0 | \psi_b^0 \rangle = 0$

↳ DUE TO PERTURBATION H'

$\downarrow$

DEGENERACY BETWEEN 2 LEVELS IS LIFTED

ASSUME $|\psi\rangle$ IS SOLUTION OF $H = H^0 + \lambda H'$

($\lambda = 1$ AT END)

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

$$|\psi\rangle = |\psi^0\rangle + \lambda |\psi^1\rangle + \lambda^2 |\psi^2\rangle + \dots$$

WITH $|\psi^0\rangle = \alpha |\psi_a^0\rangle + \beta |\psi_b^0\rangle$

$$H|\psi\rangle = E|\psi\rangle$$

$$(H^0 + \lambda H')(|\psi^0\rangle + \lambda|\psi'\rangle + \cdots)$$

$$= (E^0 + \lambda E' + \cdots)(|\psi^0\rangle + \lambda|\psi'\rangle + \cdots)$$

$\Downarrow$

0 - ORDER : $H^0|\psi^0\rangle = E^0|\psi^0\rangle$ ORIGINAL PROBLEM SOLVED !

1 - ORDER : $H^0|\psi'\rangle + H'|\psi^0\rangle = E^0|\psi'\rangle + E'|\psi^0\rangle$

TAKE $\langle\psi_a^0|$ & USE $|\psi^0\rangle = \alpha|\psi_a^0\rangle + \beta|\psi_b^0\rangle$

$$\langle\psi_a^0|H^0|\psi'\rangle + \langle\psi_a^0|H'|\psi^0\rangle$$

$$= E^0\langle\psi_a^0|\psi'\rangle + \alpha E'$$

$\Downarrow$ $\langle\psi_a^0|H^0|\psi'\rangle = E^0\langle\psi_a^0|\psi'\rangle$

$$\boxed{\alpha\langle\psi_a^0|H'|\psi_a^0\rangle + \beta\langle\psi_a^0|H'|\psi_b^0\rangle = \alpha E'}$$

NOTE : IF $\beta = 0$, $\alpha = 1$ WE FIND BACK FIRST ORDER FORMULA IN NON-DEGENERATE CASE

↳ INTRODUCE 'TRANSITION MATRIX ELEMENTS'

$$\boxed{W_{ij} \equiv \langle \psi_i^0 | H' | \psi_j^0 \rangle}$$

KNOWN ONCE WE SOLVED FOR $|\psi_i^0\rangle$

1- ORDER FORMULA $\alpha E' = \alpha W_{aa} + \beta W_{ab}$ (*)

IF TAKING CONTRACTION WITH $\langle \psi_b^0 |$ INSTEAD,

WE FIND AN ANALOGOUS FORMULA ($a \leftrightarrow b$)

$$\beta E' = \beta W_{bb} + \alpha W_{ba} \quad (**)$$

(**) $\cdot$ W_{ab}

$$(\beta W_{ab}) E' = (\beta W_{ab}) W_{bb} + \alpha |W_{ab}|^2$$

↓ USE (*) FOR βW_{ab}

$$(\alpha E' - \alpha W_{aa})(E' - W_{bb}) = \alpha |W_{ab}|^2$$

↓ α DROPS OUT

$$E'^2 - (W_{aa} + W_{bb}) E' + W_{aa} W_{bb} - |W_{ab}|^2 = 0$$

$$\boxed{E'_\pm = \frac{1}{2}\left[W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{ab}|^2} \right]}$$

SPECIAL CASES

$$|\psi^0\rangle = \alpha\,|\psi_a^0\rangle + \beta\,|\psi_b^0\rangle$$

$\rightsquigarrow \alpha = 1,\ \beta = 0 \quad \Rightarrow \quad W_{ba} = 0 \qquad (**)$

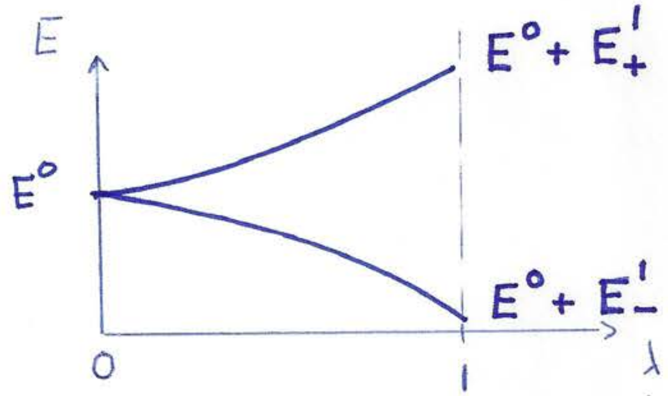
$\qquad E^1 \underset{(*)}{=} W_{aa} \overset{!}{=} E_+^1$

$\rightsquigarrow \alpha = 0,\ \beta = 1 \quad \Rightarrow \quad W_{ab} = 0 \qquad (*)$

$\qquad E^1 \underset{(**)}{=} W_{bb} \overset{!}{=} E_-^1$

IN BOTH CASES WE FIND BACK RESULTS OF NON-DEGENERATE PERTURBATION THEORY

IN GENERAL



↳ DENOTES 'SWITCHING ON' THE PERTURBATION H^1 FROM 0 TO 1

↳ USEFUL THEOREM TO DETERMINE 'GOOD' LINEAR COMBINATION TO APPLY NON-DEG. P.T.

THEOREM : A HERMITIAN OPERATOR

$$[A, H^\circ] = [A, H'] = 0$$

IF $|\psi_a^\circ\rangle$ AND $|\psi_b^\circ\rangle$ ARE ALSO EIGENFUNCTIONS OF A :

$$A|\psi_a^\circ\rangle = \mu|\psi_a^\circ\rangle$$

$$A|\psi_b^\circ\rangle = \nu|\psi_b^\circ\rangle$$

SUCH THAT $\mu \neq \nu$

$$\Downarrow$$

$W_{ab} = 0 \Rightarrow$ WE CAN APPLY NON-DEG. PT

$$E_+^1 = W_{aa} = \langle\psi_a^\circ|H'|\psi_a^\circ\rangle$$

$$E_-^1 = W_{bb} = \langle\psi_b^\circ|H'|\psi_b^\circ\rangle$$

PROOF : $0 = \langle\psi_a^\circ|[A, H']|\psi_b^\circ\rangle$

$$= \langle\psi_a^\circ|AH'|\psi_b^\circ\rangle - \langle\psi_a^\circ|H'A|\psi_b^\circ\rangle$$

$$= (\mu - \nu)\langle\psi_a^\circ|H'|\psi_b^\circ\rangle$$

$$= (\mu - \nu)\, W_{ab} \Rightarrow \text{IF } \mu \neq \nu \Rightarrow W_{ab} = 0 \quad \blacksquare$$

• MATRIX NOTATION

2 - FOLD DEGENERACY

$\hookrightarrow \quad H^0 |\psi_a^0\rangle = E^0 |\psi_a^0\rangle$

$H^0 |\psi_b^0\rangle = E^0 |\psi_b^0\rangle$

$|\psi^0\rangle = \alpha |\psi_a^0\rangle + \beta |\psi_b^0\rangle$

$\hookrightarrow \quad H = H^0 + \lambda H^1$

$E = E^0 + \lambda E^1 + \cdots$

$|\psi\rangle = |\psi^0\rangle + \lambda |\psi^1\rangle + \cdots$

$H |\psi\rangle = E |\psi\rangle$

TO FIRST ORDER IN PERTURBATION

2 EQS.
$$\begin{cases} \alpha W_{aa} + \beta W_{ab} = \alpha E^1 \\ \alpha W_{ba} + \beta W_{bb} = \beta E^1 \end{cases}$$

$\hookrightarrow$ IN MATRIX NOTATION: WITH $W_{ij} \equiv \langle \psi_i^0 | H^1 | \psi_j^0 \rangle$

$$\underbrace{\begin{pmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{pmatrix}}_{\equiv W} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E^1 \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$\therefore \quad E^1$: EIGENVALUES OF W MATRIX

(α, β) : GOOD LIN. COMB. OF UNPERTURBED STATES

$\hookrightarrow$ EIGENVECTORS OF W

• HIGHER-ORDER DEGENERACY

↳ n - FOLD DEGENERACY

$$|\psi_1^0\rangle, \; |\psi_2^0\rangle, \ldots, \; |\psi_n^0\rangle$$

ARE DEGENERATE → ENERGY E^0

↳ $n \times n$ MATRIX W

$$W_{ij} \equiv \langle \psi_i^0 | H' | \psi_j^0 \rangle$$

↳ FIRST ORDER CORRECTIONS TO ENERGY ⇒ EIGENVALUES OF W

GOOD LIN. COMB. OF UNPERTURBED STATES

⇓

EIGENVECTORS OF W

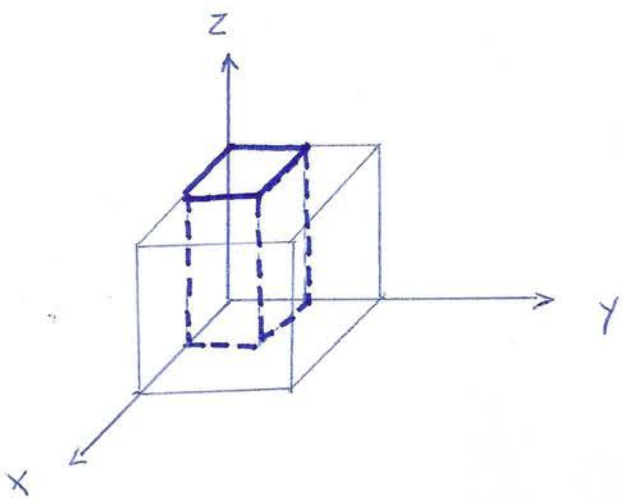
- **EXAMPLE** : 3-DIM INFINITE CUBIC WELL

WITH PERTURBATION

↳ $$H^0 = \frac{\hat{P}^2}{2m} + V(x, y, z)$$

$$V(x,y,z) = \begin{cases} 0 & , \quad 0 < x < a \\ & \quad\;\; 0 < y < a \\ & \quad\;\; 0 < z < a \\ \infty & , \quad \text{OTHERWISE} \end{cases}$$

↳ $$H^1 = \begin{cases} V_0 & , \quad 0 < x < a/2 \\ & \quad\;\; 0 < y < a/2 \\ 0 & , \quad \text{OTHERWISE} \end{cases}$$



PARTICLE FEELS PERTURBATION WHEN IT IS IN SMALLER BOX

↳ UNPERTURBED PROBLEM

$$\psi^{0}_{n_x n_y n_z}(x,y,z) = C \sin\left(n_x \frac{\pi}{a} x\right) \sin\left(n_y \frac{\pi}{a} y\right) \sin\left(n_z \frac{\pi}{a} z\right)$$

$$C = \left(\frac{2}{a}\right)^{3/2}$$

$$E^{0}_{n_x n_y n_z} = \frac{\hbar^2}{2m} \frac{\pi^2}{a^2} \left(n_x^2 + n_y^2 + n_z^2\right)$$

⤳ GROUND STATE : $n_x = n_y = n_z = 1$

NON-DEGENERATE $\quad E^{0}_{0} = \frac{\hbar^2}{2m} \frac{3\pi^2}{a^2}$

⤳ FIRST EXCITED STATE : $n_x = 1, \; n_y = 1, \; n_z = 2$

$n_x = 1, \; n_y = 2, \; n_z = 1$

$n_x = 2, \; n_y = 1, \; n_z = 1$

TRIPLY DEGENERATE

$$\psi^{0}_{a} \equiv \psi^{0}_{112}, \quad \psi^{0}_{b} \equiv \psi^{0}_{121}, \quad \psi^{0}_{c} \equiv \psi^{0}_{211}$$

ALL 3 HAVE SAME ENERGY

$$E^{0}_{1} = \frac{\hbar^2}{2m} \frac{6\pi^2}{a^2}$$

↳ PERTURBATION THEORY

$$|\psi^0\rangle \equiv \alpha\,|\psi_a^0\rangle + \beta\,|\psi_b^0\rangle + \gamma\,|\psi_c^0\rangle$$

↳ GOOD LIN. COMB OF UNPERTURBED STATES

$$W_{ij} = \langle \psi_i^0 | H' | \psi_j^0 \rangle$$

$$i, j = a, b, c$$

- $W_{aa} = W_{bb} = W_{cc}$

$$= \left(\frac{2}{a}\right)^3 V_0 \int_0^{a/2} dx\, \sin^2\left(\frac{\pi}{a}x\right) \int_0^{a/2} dy\, \sin^2\left(\frac{\pi}{a}y\right) \cdot \int_0^a dz\, \sin^2\left(\frac{2\pi}{a}z\right)$$

$$= \left(\frac{2}{a}\right)^3 V_0 \cdot \left(\frac{1}{2}\,\frac{a}{2}\right)\left(\frac{1}{2}\,\frac{a}{2}\right)\left(\frac{1}{2}\,a\right)$$

$$= \frac{V_0}{4}$$

- $$W_{ab} = \left(\frac{2}{a}\right)^3 V_0 \int_0^{a/2} dx \sin^2\left(\frac{\pi}{a}x\right)$$

$$\cdot \int_0^{a/2} dy \sin\left(\frac{\pi}{a}y\right) \sin\left(\frac{2\pi}{a}y\right)$$

$$\cdot \int_0^{a} dz \underbrace{\sin\left(\frac{2\pi}{a}z\right) \sin\left(\frac{\pi}{a}z\right)}_{\frac{1}{2}\left(\cos\frac{\pi}{a}z - \cos\frac{3\pi}{a}z\right)}$$

$$\int_0^a: \quad 0 \qquad 0$$

$$W_{ab} = W_{ac} = 0$$

- $$W_{bc} = \left(\frac{2}{a}\right)^3 V_0 \int_0^{a/2} dx \sin\left(\frac{\pi}{a}x\right) \sin\left(\frac{2\pi}{a}x\right)$$

$$\cdot \int_0^{a/2} dy \sin\left(\frac{2\pi}{a}y\right) \sin\left(\frac{\pi}{a}y\right)$$

$$\cdot \int_0^{a} dz \sin^2\left(\frac{\pi}{a}z\right)$$

$$= \left(\frac{2}{a}\right)^3 \cdot V_0 \cdot \left(\frac{1}{2}\cdot\frac{4}{3}\frac{a}{\pi}\right)\left(\frac{1}{2}\cdot\frac{4}{3}\frac{a}{\pi}\right)\cdot\left(\frac{1}{2}a\right)$$

$$= \frac{16}{9}\frac{1}{\pi^2} V_0$$

$$W = \frac{V_0}{4}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & K \\ 0 & K & 1 \end{pmatrix}$$

$$K \equiv \left(\frac{8}{3\pi}\right)^2$$

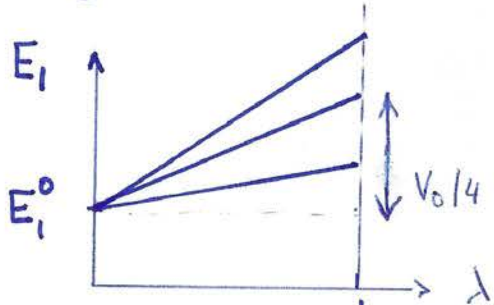
$$\begin{vmatrix} 1-w & 0 & 0 \\ 0 & 1-w & K \\ 0 & K & 1-w \end{vmatrix} = 0$$

$$\Updownarrow$$

$$(1-w)^3 - K^2(1-w) = 0$$

$$\begin{cases} w_1 = 1 & \Rightarrow \quad E_1^{(1)} = E_1^0 + \dfrac{V_0}{4} \\ w_2 = 1 + K & \Rightarrow \quad E_1^{(2)} = E_1^0 + \dfrac{V_0}{4}(1+K) \\ w_3 = 1 - K & \Rightarrow \quad E_1^{(3)} = E_1^0 + \dfrac{V_0}{4}(1-K) \end{cases}$$

UNPERTURBED ENERGIES.



- GOOD UNPERTURBED STATES

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & K \\ 0 & K & 1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = w \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}$$

$\rightsquigarrow \; w = 1 \quad \Longleftrightarrow \quad \beta = \gamma = 0 \;, \quad \alpha = 1$

$\rightsquigarrow \; w = 1 + K \quad \Longleftrightarrow \quad \alpha = 0 \;, \quad \beta = \gamma = \frac{1}{\sqrt{2}}$

$\rightsquigarrow \; w = 1 - K \quad \Longleftrightarrow \quad \alpha = 0 \;, \quad \beta = -\gamma = \frac{1}{\sqrt{2}}$

$$|\psi^0\rangle = \begin{cases} |\psi_a^0\rangle \\ \frac{1}{\sqrt{2}} \left\{ |\psi_b^0\rangle + |\psi_c^0\rangle \right\} \\ \frac{1}{\sqrt{2}} \left\{ |\psi_b^0\rangle - |\psi_c^0\rangle \right\} \end{cases}$$

$\downarrow$

CORRESPOND WITH 3 STATES.

• FIRST - ORDER CORRECTION TO STATES

E_m^0 ═══ } d_m FOLD DEGENERATE

E_n^0 ═══ } d_n FOLD DEGENERATE ⇒ STATES $|\psi_{n,1}^0\rangle$,
$|\psi_{n,2}^0\rangle$,
....
$|\psi_{n,d_n}^0\rangle$

GOOD UNPERTURBED STATES

$$\boxed{|\psi_{n_i}^0\rangle = \sum_{j=1}^{d_n} \alpha_{ij} \, |\psi_{n,j}^0\rangle}$$

↳ $i = 1 \ldots d_n$

* FIRST ORDER EQ. FOR STATE n_i $(i = 1 \ldots d_n)$

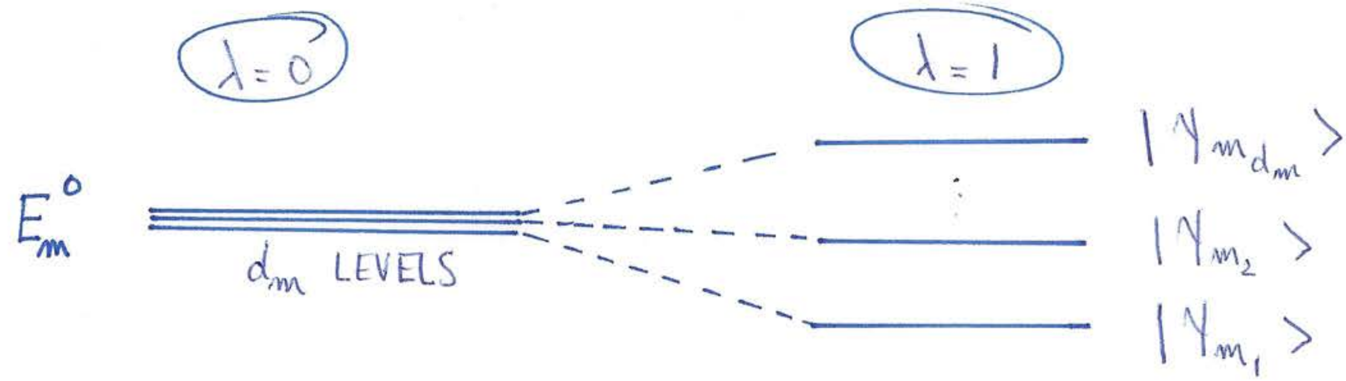
$$H^0 |\psi_{n_i}^1\rangle + H^1 |\psi_{n_i}^0\rangle = E_n^0 |\psi_{n_i}^1\rangle + E_{n_i}^1 |\psi_{n_i}^0\rangle$$

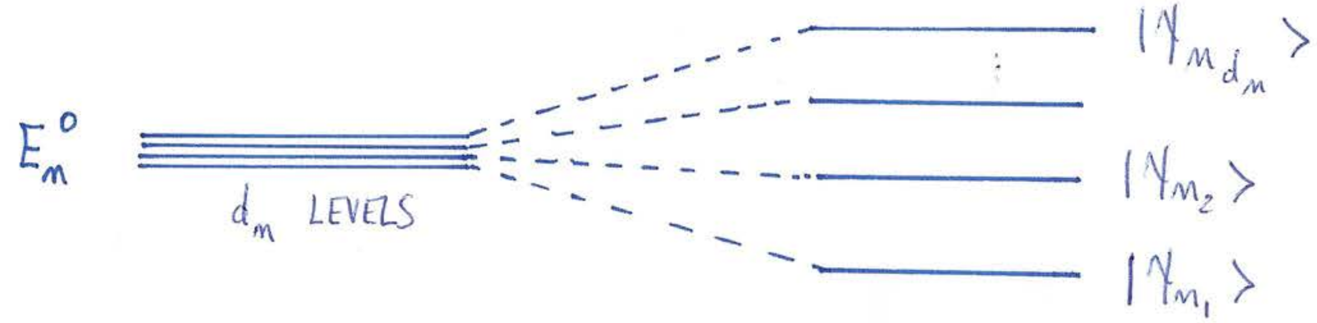
↓

$|\psi_{n_i}^1\rangle$ CAN BE EXPANDED IN COMPLETE BASIS

$$\boxed{(H^0 - E_n^0) |\psi_{n_i}^1\rangle = (E_{n_i}^1 - H^1) |\psi_{n_i}^0\rangle}$$

$$|\psi^1_{n_i}\rangle = \sum_{m \neq n} \sum_{j=1}^{d_m} c_{n_i m_j} \, |\psi^0_{m_j}\rangle$$





$$(H^0 - E_n^0) \sum_{m \neq n} \sum_{j=1}^{d_m} c_{n_i m_j} \, |\psi^0_{m_j}\rangle$$

$$= (E^1_{n_i} - H') \, |\psi^0_{n_i}\rangle$$

$$\Downarrow$$

$$\sum_{m \neq n} \left(E_m^\circ - E_n^\circ \right) \sum_{j=1}^{d_m} c_{n_i m_j} \ |\psi_{m_j}^\circ\rangle$$

$$= \left(E_{n_i}^1 - H' \right) |\psi_{n_i}^\circ\rangle$$

$$\Downarrow \qquad \langle \psi_{m_k}^\circ | \qquad m \neq n$$

$$\left(E_m^\circ - E_n^\circ \right) \sum_{j=1}^{d_m} c_{n_i m_j} \underbrace{\langle \psi_{m_k}^\circ | \psi_{m_j}^\circ \rangle}_{\delta_{jk}}$$

$$= \langle \psi_{m_k}^\circ | (\cancel{E_{n_i}^1} - H') |\psi_{n_i}^\circ\rangle$$

$$m \neq n$$

$$\left(E_m^\circ - E_n^\circ \right) c_{n_i m_k} = - \langle \psi_{m_k}^\circ | H' | \psi_{n_i}^\circ \rangle$$

$$\boxed{|\psi_{n_i}^1\rangle = \sum_{m \neq n} \sum_{j=1}^{d_m} \frac{\langle \psi_{m_j}^\circ | H' | \psi_{n_i}^\circ \rangle}{E_n^\circ - E_m^\circ} \cdot |\psi_{m_j}^\circ\rangle}$$

⇒ FINE STRUCTURE OF HYDROGEN

- BOHR THEORY FOR H: $E_n = \frac{E_1}{n^2}$

$$E_1 = -\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 = -13.6\ eV$$

$$\Downarrow \qquad \boxed{\alpha \equiv \frac{e^2}{4\pi\varepsilon_0 \hbar c} \simeq \frac{1}{137}}$$

↳ FINE STRUCTURE CONSTANT
DIMENSIONLESS PARAMETER WHICH DENOTES STRENGTH OF ELECTROMAGNETIC INTERACTION

$$\boxed{E_1 = -\frac{\alpha^2}{2} mc^2}$$

- FINE - STRUCTURE CORRECTIONS TO E_n

1) RELATIVISTIC CORRECTIONS

2) SPIN - ORBIT COUPLING

SPIN 1/2 IS COUPLED WITH ORBITAL ANGULAR MOMENTUM $\bar{\ell}$ TO TOTAL ANGULAR MOMENTUM $\bar{J}$

• RELATIVISTIC CORRECTIONS

↳ NON REL. $p = mv$

KIN. EN. : $T = \frac{1}{2} m v^2 = \frac{p^2}{2m}$

↳ REL. $p = m_{rel} v$

$$m_{rel} = \frac{m}{\sqrt{1 - v^2/c^2}}$$

RELATIVISTIC MASS

RESTMASS : MASS IN FRAME WHERE $v = 0$

TOTAL ENERGY (OF FREE PARTICLE) $E = m_{rel} c^2$ (EINSTEIN FORMULA)

$$= \frac{m}{\sqrt{1 - v^2/c^2}} c^2$$

KINETIC ENERGY OF PARTICLE MOVING WITH VELOCITY v

$$T = E - \underbrace{mc^2}_{\text{REST ENERGY}}$$

(WHEN PARTICLE IS AT REST $v = 0 \Rightarrow T = 0$)

$$T = m_{rel}\, c^2 - mc^2$$

$$= \frac{m}{\sqrt{1 - v^2/c^2}}\, c^2 - mc^2$$

$$\hookrightarrow \quad E^2 = \frac{m^2 c^4}{1 - v^2/c^2}$$

$$= \frac{1}{1 - v^2/c^2} \left\{ 1 - \frac{v^2}{c^2} + \frac{v^2}{c^2} \right\} m^2 c^4$$

$$= \frac{v^2/c^2}{1 - v^2/c^2} \cdot m^2 c^4 + m^2 c^4$$

$$= \frac{m^2}{1 - v^2/c^2}\, v^2 c^2 + m^2 c^4$$

$$\boxed{E^2 = c^2 p^2 + m^2 c^4} \quad \Rightarrow \quad E = \sqrt{c^2 p^2 + m^2 c^4}$$

$$\hookrightarrow \quad T = E - mc^2$$

$$= \sqrt{c^2 p^2 + m^2 c^4} - mc^2$$

FOR A NONREL. SYSTEM

$$\underline{v \ll c} \quad \text{(} e^- \text{ MOVES WITH VELOCITY MUCH SMALLER THAN VELOCITY OF LIGHT)}$$

$$\Updownarrow$$

$$p \ll mc$$

(FOR H OK ! $\langle T \rangle \simeq 10 \text{ eV}$

$mc^2 \simeq 511 \text{ keV}$

$$\frac{\langle T \rangle}{mc^2} \simeq 0.2 \; 10^{-4} \;)$$

EXPAND RELATIVISTIC KINETIC ENERGY

$$T = \sqrt{m^2c^4 + c^2p^2} - mc^2$$

$$= mc^2 \sqrt{1 + \frac{p^2}{m^2c^2}} - mc^2$$

$$= mc^2 \left(1 + \frac{p^2}{2m^2c^2} - \frac{1}{8} \left(\frac{p^2}{m^2c^2} \right)^2 + O(p^6) \right) - mc^2$$

$$\boxed{T = \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \cdots}$$

NONREL. KIN. EN   RELATIVISTIC CORRECTION

↳ CONSIDER RELATIVISTIC CORRECTION AS PERTURBATION

$$H^0 = \frac{\hat{p}^2}{2m} \underbrace{- \frac{\alpha \hbar c}{r}}_{\hat{V}}$$

$$H^1_{rel} = - \frac{\hat{p}^4}{8m^3c^2}$$

1° ORDER PERTURBATION THEORY : APPLY NON-DEG. PT

$$E^1_{rel} = \langle \psi^0 | H^1_{rel} | \psi^0 \rangle$$

$$\left\{ \begin{array}{l} [L^2, H^1] = 0 \\ [L_z, H^1] = 0 \\ \text{PERT. IS SPHERICAL SYMM.} \end{array} \right.$$

↑ REL. CORRECTION TO H-ATOM ENERGIES

UNPERTURBED H-ATOM WAVE FUNCTIONS

$$E^1_{rel} = - \frac{1}{8m^3c^2} \langle \psi^0 | \hat{p}^4 | \psi^0 \rangle$$

$$= - \frac{1}{8m^3c^2} \langle \hat{p}^2 \psi^0 | \hat{p}^2 \psi^0 \rangle$$

$$\Downarrow \quad \frac{\hat{p}^2}{2m} \psi^0 = (E - \hat{V}) \psi^0$$

$$E'_{rel} = -\frac{1}{2mc^2} \langle \psi^0 | (E - \hat{V})^2 | \psi^0 \rangle$$

$$= -\frac{1}{2mc^2} \left\{ E^2 - 2E \langle \hat{V} \rangle + \langle \hat{V}^2 \rangle \right\}$$

$$\Downarrow \qquad \hat{V} = -\frac{\alpha \hbar c}{r}$$

$$\boxed{E'_{rel} = -\frac{1}{2mc^2} \left\{ E_n^2 + 2E_n \alpha \hbar c \left\langle \frac{1}{r} \right\rangle + \alpha^2 (\hbar c)^2 \left\langle \frac{1}{r^2} \right\rangle \right\}}$$

FOR LEVEL n

↳ EVALUATE $\left\langle \frac{1}{r} \right\rangle$, $\left\langle \frac{1}{r^2} \right\rangle$

IN STATE $\psi^0 = \underbrace{\psi_{n\ell m}}$

H-ATOM UNPERTURBED WAVE FUNCTIONS.

$$\psi_{100} = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$$

BOHR RADIUS $\boxed{a = \left(\frac{4\pi\varepsilon_0}{e^2} \right) \frac{\hbar^2}{m} = \frac{1}{\alpha m} \frac{\hbar}{c}}$

$\hookrightarrow$ USE FEYNMAN - HELLMANN THEOREM

TO EVALUATE $\langle \frac{1}{r} \rangle$, $\langle \frac{1}{r^2} \rangle$ IN GENERAL STATE $\psi_{n\ell m}$

FEYNMAN HELLMANN THEOREM !

IF H DEPENDS ON SOME PARAMETER λ

$\hookrightarrow$ $E_n(\lambda)$, $\psi_n(\lambda)$ EIGENVALUES, EIGENFUNCTIONS OF $H(\lambda)$

$\Downarrow$

$$\boxed{\frac{\partial E_n}{\partial \lambda} = \langle \psi_n | \frac{\partial H}{\partial \lambda} | \psi_n \rangle}$$

PROOF : WE CAN ASSUME

EITHER NON-DEGENERATE

OR ψ_n GOOD LIN. COMB. OF DEGENERATE EIGENSTATES

INFINITESIMAL CHANGE TO λ

$$\lambda = \lambda_0 + d\lambda \qquad H(\lambda) = H(\lambda_0) + d\lambda \left.\frac{\partial H}{\partial \lambda}\right|_{\lambda_0} + O(d\lambda)^2$$

1° ORDER CORRECTION TO ENERGY

$$\underset{\displaystyle d\lambda \frac{\partial E_n}{\partial \lambda}}{\underset{\shortparallel}{dE_n}} \simeq \langle \psi_n | \underbrace{H'}_{d\lambda \left.\frac{\partial H}{\partial \lambda}\right|_{\lambda_0}} | \psi_n \rangle$$

$$\therefore \quad \frac{\partial E_n}{\partial \lambda} = \langle \psi_n | \frac{\partial H}{\partial \lambda} | \psi_n \rangle$$

↳ RADIAL SCHRÖDINGER EQ. FOR H- ATOM

$$H^\circ = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \underbrace{\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}}_{\text{'CENTRIFUGAL' TERM}} - \frac{\alpha\hbar c}{r}$$

↓

EIGENVALUES $\quad E_n = -\left(\frac{1}{2} mc^2 \alpha^2\right)\frac{1}{n^2}$

* APPLY FEYNMAN - HELLMANN THEOREM FOR $\lambda = \alpha$

$$\frac{\partial H^0}{\partial \alpha} = -\frac{\hbar c}{r}$$

$$\frac{\partial E_n}{\partial \alpha} = -\frac{\alpha m c^2}{n^2}$$

⇓

$$\boxed{\left\langle \frac{1}{r}\right\rangle = \frac{\alpha m c^2}{\hbar c}\frac{1}{n^2} = \frac{1}{a n^2}}$$

$$= -\frac{2E_n}{\alpha\hbar c}$$

6.32

* APPLY FEYNMAN - HELLMANN THEOREM FOR $\lambda = \ell$

$$\left\langle \frac{\partial H^0}{\partial \ell} \right\rangle = \frac{\hbar^2}{m} \left\langle \frac{1}{r^2} \right\rangle \left(\ell + \frac{1}{2}\right)$$

$$E_n = + \frac{E_1}{(j_{max} + \ell + 1)^2}$$

$$n = \underset{\substack{\uparrow \\ \text{INTEGER}}}{j_{max}} + \ell + 1$$

$$\frac{\partial E_n}{\partial \ell} = - \frac{2 E_1}{n^3} = - \frac{2n}{E_1} \cdot E_n^2$$

$$\left\langle \frac{1}{r^2} \right\rangle = - \frac{2 E_1 \, m}{\hbar^2} \, \frac{1}{\left(\ell + \frac{1}{2}\right) n^3}$$

$$\downarrow \qquad -E_1 = \frac{1}{2} m c^2 \alpha^2$$

$$\boxed{\left\langle \frac{1}{r^2} \right\rangle = \frac{1}{a^2} \, \frac{1}{\left(\ell + \frac{1}{2}\right) n^3}}$$

$$\therefore \quad E^1_{rel} = -\frac{1}{2mc^2}\left\{ E_n^2 + 2E_n \alpha \hbar c \frac{1}{an^2} + \alpha^2 \hbar^2 c^2 \frac{1}{a^2(l+\frac{1}{2})n^3} \right\}$$

$$\downarrow \quad E_n = -\left(\frac{1}{2} mc^2 \alpha^2\right)\frac{1}{n^2}$$

$$\frac{1}{an^2} = \alpha m \frac{c}{\hbar}\frac{1}{n^2} = -\frac{2E_n}{\hbar c}\frac{1}{\alpha}$$

$$E^1_{rel} = -\frac{1}{2mc^2}\left\{ E_n^2 - (2E_n)\cdot(2E_n) + \frac{n}{(l+\frac{1}{2})} 4E_n^2 \right\}$$

$$\boxed{E^1_{rel} = -\frac{E_n^2}{2mc^2}\left\{ -3 + \frac{4n}{l+1/2} \right\}}$$

DEPENDS ON n AND l!

SIZE: $\frac{E_n^2}{2mc^2} \simeq \frac{(13.6\text{ eV})^2}{1.022\times 10^6\text{ eV}} \simeq 1.8\ 10^{-4}\text{ eV}$

OF ORDER $\alpha^2 \sim 10^{-4}$ RELATIVE TO E_n

↳ $n = 1$, $l = 0$

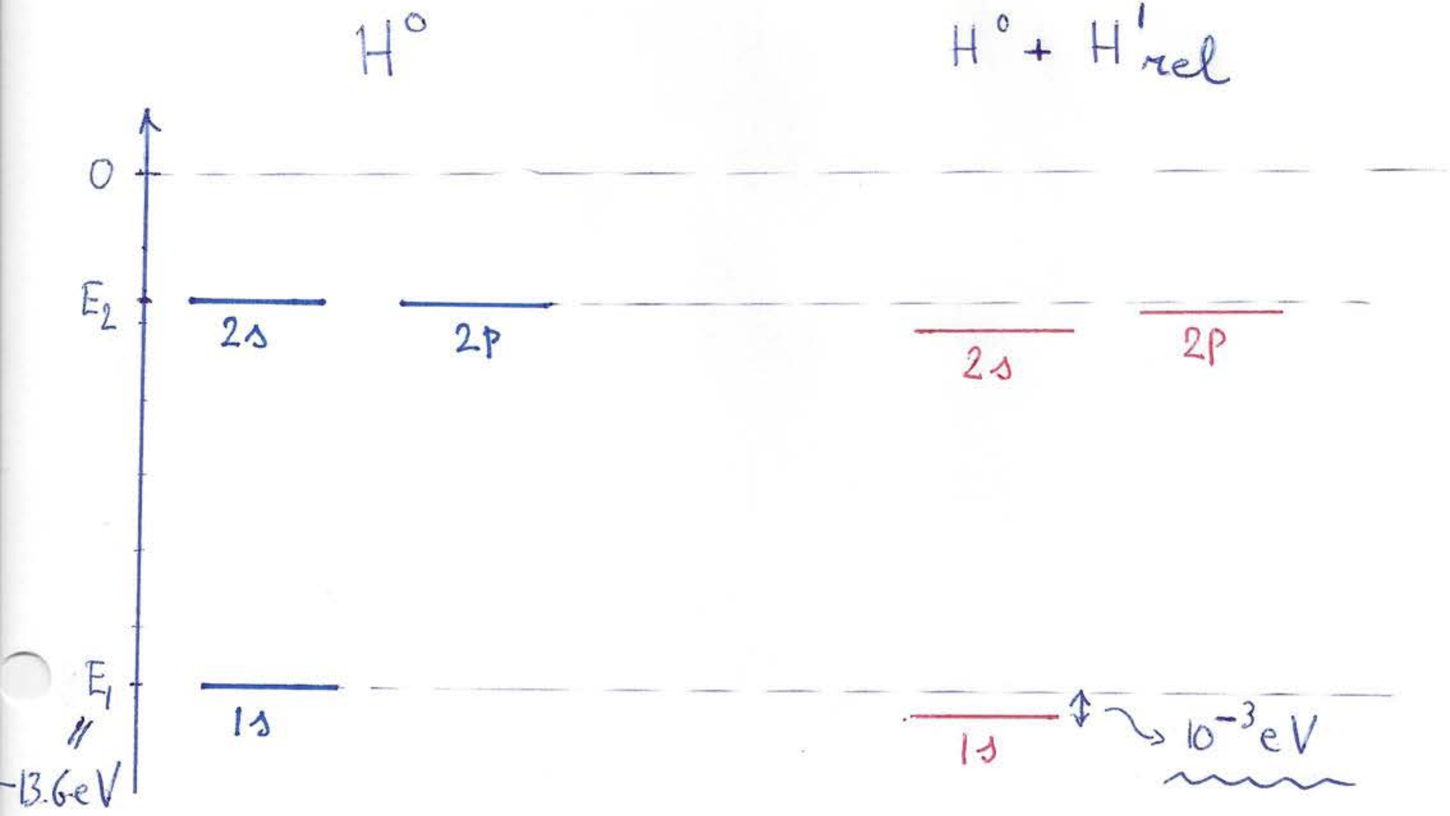
$$E^1_{rel} = -\frac{E_1^2}{2mc^2}\left\{-3 + \frac{4}{1/2}\right\}$$

$$= -\frac{E_1^2}{2mc^2} \cdot 5 \simeq 10^{-3}\,eV$$

↳ $n = 2$

$l = 0 \rightarrow$ $$E^1_{rel} = -\frac{E_2^2}{2mc^2}\underbrace{\left\{-3 + 16\right\}}_{13}$$

$l = 1 \longrightarrow$ $$E^1_{rel} = -\frac{E_2^2}{2mc^2}\underbrace{\left\{-3 + \frac{16}{3}\right\}}_{7/3}$$



SPIN - ORBIT COUPLING

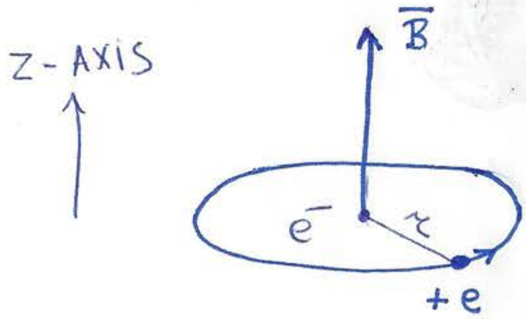
↳ IN e^- REFERENCE FRAME

↓

PROTON (CHARGE $+e$) IS CIRCLING AROUND IT

↓

CURRENT LOOP CREATES A MAGN. FIELD $\bar{B}$
WHICH INTERACTS WITH MAGN. MOMENT $\bar{\mu}$ OF e^-



↳ $\bar{B}$ FIELD CREATED BY PROTON

CURRENT $I = \dfrac{e}{T}$ $\quad$ T = PERIOD OF ORBIT

$v = \dfrac{2\pi r}{T}$

$\bar{B}$ - FIELD AT CENTER OF LOOP

$$\bar{B} = \frac{\mu_0 \, I}{2r} \bar{e}_z \text{ (BIOT-SAVART)} \quad \varepsilon_0 \mu_0 = \frac{1}{c^2}$$

e^- ORBITAL ANGULAR MOM. IN REST FRAME OF P

$$\bar{L} = m v r \, \bar{e}_z = \frac{2\pi m r^2}{T} \bar{e}_z$$

$$\bar{B} = \frac{\mu_0 e}{2r T} \bar{e}_z$$

$$= \frac{\mu_0 e}{4\pi r^3 m} \underbrace{\left(\frac{2\pi m r^2}{T}\right) \bar{e}_z}_{\bar{L}}$$

$$\boxed{\bar{B} = \frac{e}{4\pi \varepsilon_0 c^2} \frac{1}{m r^3} \bar{L}}$$

↳ $\bar{\mu}$ OF e^-

$$\bar{\mu} = \gamma \bar{S}$$

CLASSICAL $\quad \gamma = \frac{q}{2m} \underset{\uparrow}{=} -\frac{e}{2m}$

FOR e^-

QUANTUM $\quad \gamma = \underset{\uparrow}{g} \frac{q}{2m}$

g- FACTOR

DIRAC THEORY (RELATIVISTIC QM)

EXPLAINS $\underline{\underline{g = 2}}$! FOR SPIN 1/2. POINT PARTICLE

$$\therefore \quad \boxed{\bar{\mu}_e = -\frac{2e}{2m}\bar{S} = -\frac{e}{m}\bar{S}}$$

↳ SPIN-ORBIT INTERACTION

$$H'_{SO} = -\bar{\mu}_e \cdot \bar{B}$$

$$= +\frac{e}{m}\frac{e}{4\pi\varepsilon_0 c^2}\frac{1}{m r^3}\bar{L}\cdot\bar{S}$$

$$\boxed{H'_{SO} = \frac{1}{2}\alpha\frac{\hbar}{c}\frac{1}{m^2 r^3}\bar{L}\cdot\bar{S}}$$

IF ONE DOES THE CORRECT RELATIVISTIC CALCULATION

(THOMAS PRECESSION:

BECAUSE e^- REST FRAME IS NOT INERTIAL

↓

ACCELERATES AS e^- ORBITS p

INTERACTION DEPENDS ON VALUE OF

TOTAL ANGULAR MOMENTUM $\bar{J} = \bar{L} + \bar{S}$

$$\bar{L}\cdot\bar{S} = \frac{1}{2}\left(J^2 - L^2 - S^2\right)$$

EIGENVALUES

$$\hookrightarrow \frac{\hbar^2}{2}\left(j(j+1) - \ell(\ell+1) - \frac{3}{4}\right)$$

GOOD EIGENSTATES ARE

EIGENSTATES OF J^2, J_z, L^2, S^2.

(L_z, S_z DO <u>NOT</u> COMMUTE WITH H'_{SO})

$\therefore$ "GOOD" UNPERTURBED STATES $|\psi^0\rangle = |\underbrace{\psi_{n j m_j l s}}_{\text{5 QUANTUM NUMBERS}}\rangle$

5 QUANTUM NUMBERS : n, j, m_j, l, s

$\hookrightarrow$ CORRECTION TO ENERGY DUE TO S.O.

$$E^1_{SO} = \langle \psi_{n j m_j l s} | H'_{SO} | \psi_{n j m_j l s} \rangle$$

$$= \frac{1}{2} \alpha \frac{\hbar}{c} \frac{1}{m^2} \frac{\hbar^2}{2} \left[j(j+1) - l(l+1) - \frac{3}{4} \right] \cdot \left\langle \frac{1}{r^3} \right\rangle$$

PROBLEM 6.35 c) USING $\langle \frac{1}{r^2} \rangle$

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{l(l+\frac{1}{2})(l+1)} \frac{1}{n^3 a^3}$$

$$\frac{1}{n^3 a^3} = \frac{n}{a}\left(\frac{1}{n^2 a}\right)^2$$

$$= \frac{n}{a}\,\frac{4E_n^2}{\hbar^2 c^2}\,\frac{1}{\alpha^2}$$

$$\frac{1}{a} = \alpha m \frac{c}{\hbar}$$

$$= n\,\frac{4E_n^2\, m}{\hbar^3 c\,\alpha}$$

$$\therefore\; E^1_{so} = \frac{\alpha}{2}\,\frac{\hbar^3}{2m^2 c}\cdot\frac{4E_n^2\, m}{\hbar^3 c\,\alpha}\cdot n\,\frac{\left[j(j+1) - \ell(\ell+1) - \frac{3}{4}\right]}{\ell\left(\ell+\frac{1}{2}\right)(\ell+1)}$$

$$\boxed{E^1_{so} = \frac{E_n^2}{mc^2}\, n \cdot \frac{\left[j(j+1) - \ell(\ell+1) - \frac{3}{4}\right]}{\ell\left(\ell+\frac{1}{2}\right)(\ell+1)}}$$

$O(\alpha^4)$

DEPENDS ON n, j, ℓ !

- TOTAL FINE STRUCTURE CORRECTION

$$E^1_{FS} = E^1_{rel} + E^1_{SO}$$

$$= \frac{E_n^2}{2mc^2}\left\{ 3 - \frac{4n}{l+1/2} - \frac{2n}{l+1/2} + 2n\frac{\left[j(j+1)-\frac{3}{4}\right]}{l(l+1)(l+\frac{1}{2})}\right\}$$

$\hookrightarrow$ $j = l \pm 1/2 \Rightarrow l = j \mp \frac{1}{2}$

$\underset{\sim\sim\sim}{l = j - \frac{1}{2}}$: $l(l+1)(l+\frac{1}{2}) = (j+\frac{1}{2})(j-\frac{1}{2})j$

$$\{\ \} = 3 - \frac{6n}{j} + 2n\frac{\cancel{(j-\frac{1}{2})}(j+\frac{3}{2})}{(j+\frac{1}{2})\cancel{(j-\frac{1}{2})}j}$$

$$= 3 - \frac{2n}{j(j+1/2)}\left[3(j+\tfrac{1}{2}) - (j+\tfrac{3}{2})\right]$$

$$= 3 - \frac{4n}{j+1/2}$$

$\underline{l = j + \frac{1}{2}}$: $l(l+1)(l+\frac{1}{2}) = (j+\frac{1}{2})(j+\frac{3}{2})(j+1)$

$$\{\ \} = 3 - \frac{6n}{j+1} + 2n \frac{(j-\frac{1}{2})\cancel{(j+\frac{3}{2})}}{(j+\frac{1}{2})\cancel{(j+\frac{3}{2})}(j+1)}$$

$$= 3 - \frac{2n}{(j+\frac{1}{2})(j+1)} \underbrace{\left[3(j+\frac{1}{2}) - (j-\frac{1}{2})\right]}_{2j+2}$$

$$= 3 - \frac{4n}{j+\frac{1}{2}}$$ SAME RESULT !

$\therefore$

$$\boxed{\begin{aligned} E'_{FS} &= E'_{rel} + E'_{SO} \\ &= \frac{E_n^2}{2mc^2} \cdot \left\{ 3 - \frac{4n}{j+\frac{1}{2}} \right\} \end{aligned}}$$

↑

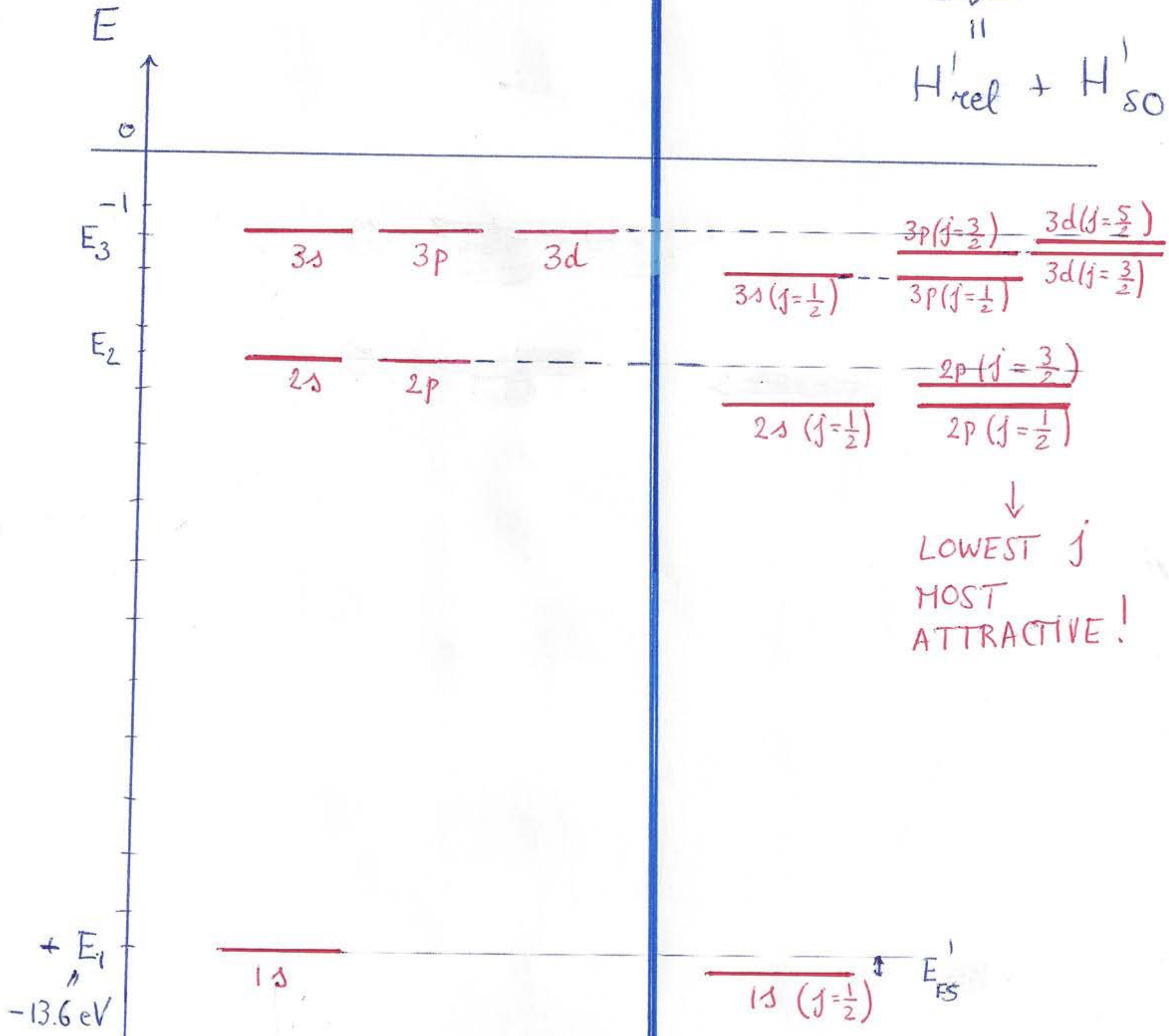
DEPENDS ONLY
ON $\underline{\underline{n\ \&\ j}}$!

ex $n = 1$
$l = 0 \Rightarrow j = \frac{1}{2}$ $\quad E'_{FS} = \frac{E_n^2}{2mc^2}\{-1\}$.

FINE - STRUCTURE OF H

H^0 (BOHR MODEL)

$$H^0 + \underbrace{H'_{FS}}_{=\ H'_{rel} + H'_{SO}}$$



TOTAL E

$$\boxed{E = E_n + E'_{FS} = -\frac{13.6\,\text{eV}}{n^2}\left[1 + \frac{\alpha^2}{n^2}\left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right)\right]}$$

DEPENDS ON n & j

⇒ ZEEMAN EFFECT (ZEEMAN 1897!)

- ATOM IN EXTERNAL MAGNETIC FIELD $\bar{B}_{ext}$

e^- ORBITAL MAGN MOMENT $\bar{\mu}_\ell$

e^- SPIN MAGN MOMENT $\bar{\mu}_s$

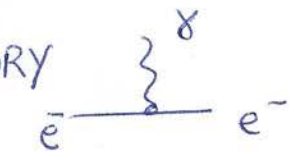
$$\underset{\substack{\uparrow \\ \text{INTERACTION} \\ \text{(ZEEMAN INTERACTION)}}}{H'_z} = -\left(\bar{\mu}_\ell + \bar{\mu}_s\right) \cdot \bar{B}_{ext}$$

$$\bar{\mu}_\ell = \gamma_\ell \, \bar{L} \qquad \gamma_\ell = -\frac{e}{2m}$$

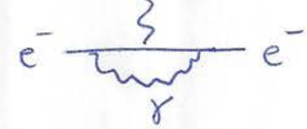
$$\bar{\mu}_s = \gamma_s \, \bar{S} \qquad \gamma_s = -\underset{\substack{\uparrow \\ \text{g- FACTOR.}}}{g} \frac{e}{2m}$$

⇒ DIRAC THEORY

$g = 2$



⇒ QUANTUM ELECTRODYNAMICS



VACUUM FLUCTUATION CORRECTIONS

$g = 2.0023$

EXPERIMENT: $g = \overbrace{2.0023193043718}^{\text{11 DIGITS !}} \pm 0.000000000000076$

FOR $g = 2$

$$\boxed{H'_z = \frac{e}{2m}\left(\bar{L} + 2\bar{S}\right).\bar{B}_{ext}}$$

↳ 3 POSSIBLE REGIMES

① IF H'_{z} IS A PERTURBATION COMPARED TO H'_{FS}

$B_{ext} << B_{int}$

↳ INTERNAL MAGN FIELD DUE TO ORBITAL MOTION OF e^- RELATIVE TO p

$$\bar{B}_{int} = \frac{e}{4\pi\varepsilon_0 c^2} \cdot \frac{1}{m r^3} \bar{L}$$

WEAK FIELD ZEEMAN EFFECT

② IF $B_{int} << B_{ext}$

TREAT H'_{FS} AS PERTURBATION TO H'_Z

③ IF $B_{int} \simeq B_{ext}$

APPLY DEGENERATE PERT. THEORY

↳ DIAGONALIZE HAMILTONIAN

• WEAK FIELD ZEEMAN EFFECT

↳ $H'_Z \ll H'_{FS}$

GOOD UNPERTURBED STATES $\underbrace{|n\,l s j\, m_j\rangle}$

GOOD QUANTUM NUMBERS FOR H'_{FS}

⇑

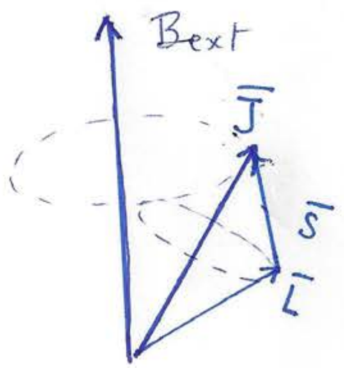
COMMUTES WITH J^2, J_z.

↳ $$E'_Z = \langle n l j m_j | H'_Z | n l j m_j \rangle$$

$$= \frac{e}{2m} \bar{B}_{ext} \cdot \langle n l j m_j | \bar{L} + 2\bar{S} | n l j m_j \rangle$$

$$\downarrow \quad \bar{J} = \bar{L} + \bar{S}$$

$$= \frac{e}{2m} \bar{B}_{ext} \cdot \langle n l j m_j | \bar{J} + \bar{S} | n l j m_j \rangle$$



$\bar{J}$ PRECESSES AROUND B_{ext} : $\omega_1 \sim B_{ext}$

$\bar{L}, \bar{S}$ PRECESS AROUND $\bar{J}$: $\omega_2 \sim B_{int}$

FOR $B_{int} \gg B_{ext}$ $\omega_2 \gg \omega_1$

FOR $\omega_2 \gg \omega$,

WE CAN REPLACE $\bar{S}$ BY ITS TIME AVERAGE

PROJECTION ALONG $\bar{J}$

$$\bar{S}_{av} = \frac{(\bar{S}.\bar{J})}{J^2} \bar{J}$$

$$\boxed{E_z' \simeq \frac{e}{2m} \bar{B}_{ext} \cdot \langle n l j m_j | \left(1 + \frac{\bar{S}.\bar{J}}{J^2} \right) \bar{J} | n l j m_j \rangle}$$

$$L^2 = (\bar{J} - \bar{S})^2$$

$$= J^2 + S^2 - 2 \bar{J}.\bar{S}$$

$$\bar{S}.\bar{J} = \frac{1}{2} (J^2 - L^2 + S^2)$$

$$\langle n l j m_j | \bar{S}.\bar{J} | n l j m_j \rangle = \frac{\hbar^2}{2} \left[j(j+1) - l(l+1) + \frac{3}{4} \right]$$

$$\boxed{E_z' \simeq \frac{e}{2m} \cdot \left[1 + \frac{j(j+1) - l(l+1) + 3/4}{2 j (j+1)} \right] \bar{B}_{ext} \cdot \langle n l j m_j | \bar{J} | n l j m_j \rangle}$$

$\downarrow$

CHOOSE Z-AXIS ALONG $\overline{B}_{ext} = B_{ext}\,\hat{e}_z$

$\rightsquigarrow$ $\langle n l j m_j \,|\, J_z \,|\, n l j m_j \rangle = \hbar m_j$

$\rightsquigarrow$ INTRODUCE <u>BOHR MAGNETON</u>

$$\boxed{\mu_B \equiv \frac{e\hbar}{2m} \simeq 5.79 \times 10^{-5}\ \frac{eV}{T}}$$

$$\boxed{E_Z' \simeq \mu_B \cdot g_j\ B_{ext} \cdot m_j}$$

LANDÉ g - FACTOR

$$\boxed{g_j \equiv 1 + \frac{j(j+1) - \ell(\ell+1) + 3/4}{2j(j+1)}}$$

DEFINES A MAGN. MOMENT $\overline{\mu}_j$ ASSOCIATED WITH $\overline{J}$

$$E_Z' = -\langle \mu_j \rangle B_{ext}$$

g-FACTOR

$$\mu_j = -\frac{e}{2m} \cdot g_j \cdot J_z$$

Z-COMPONENT OF $\overline{\mu}_j$

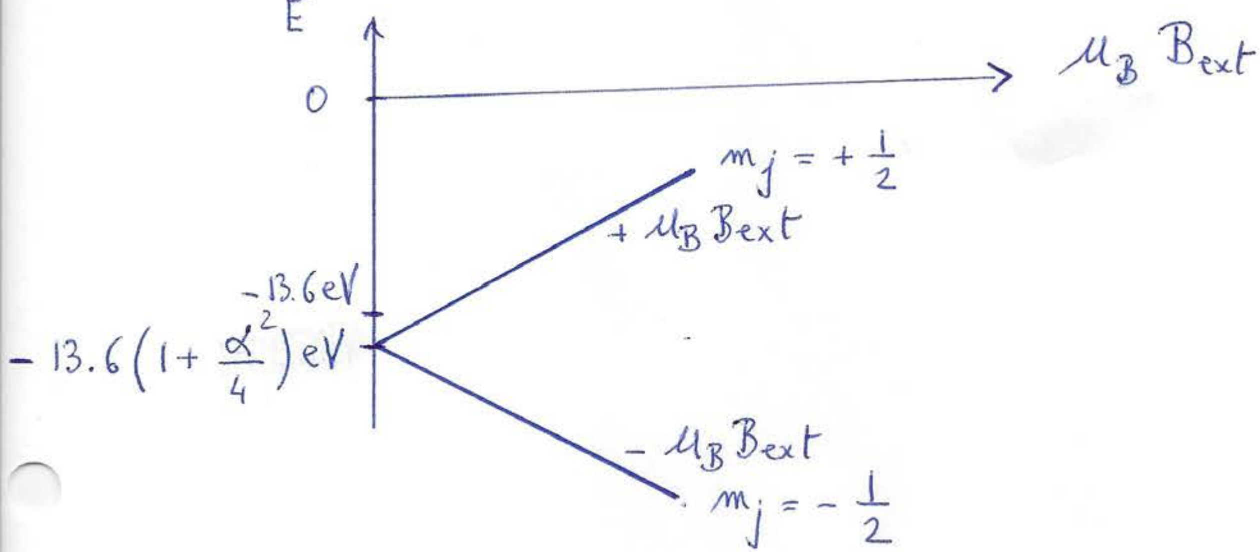
↳ GRAPHICALLY

$$\Rightarrow \boxed{n = 1,\ \ell = 0,\ j = \tfrac{1}{2},\ m_j = \pm\tfrac{1}{2}}$$ (H-ATOM GROUND STATE)

↓ SPLITS IN 2 !

$$g_{\frac{1}{2}} = 2$$

$$E_Z^1 \simeq \pm \mu_B B_{ext}$$

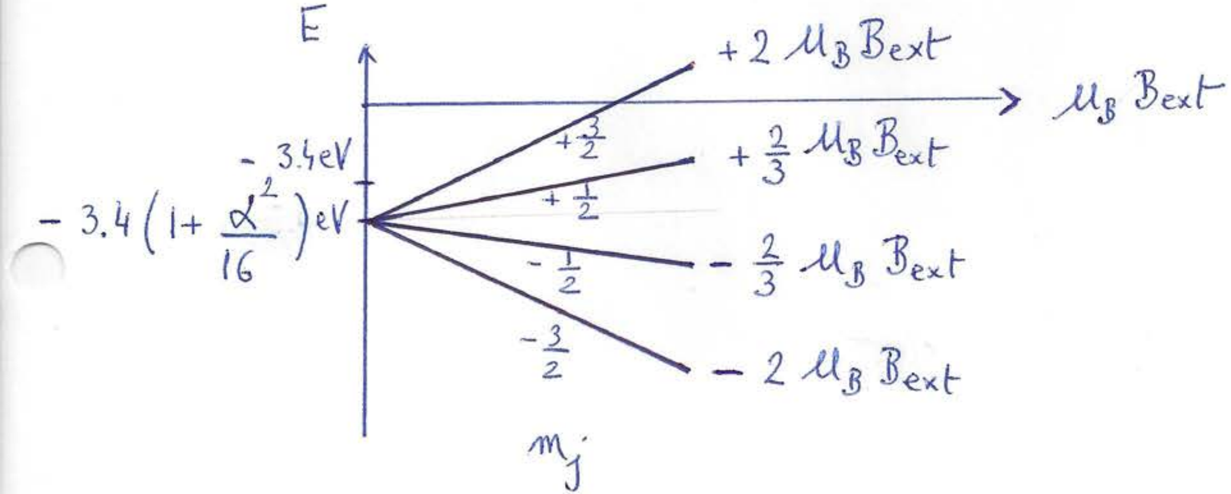


$$\Rightarrow \boxed{n = 2,\ \ell = 1,\ j = \tfrac{3}{2},\ m_j = -\tfrac{3}{2}, -\tfrac{1}{2}, +\tfrac{1}{2}, +\tfrac{3}{2}}$$

↓ SPLITS IN 4 !

$$g_{\frac{3}{2}} = \frac{4}{3}$$

$$E_Z^1 = \mu_B B_{ext} \frac{4}{3} m_j$$



• STRONG FIELD ZEEMAN EFFECT

↳ ALSO KNOWN AS PASCHEN-BACK EFFECT

$$B_{ext} \gg B_{int}$$

$$H'_Z \gg H'_{FS}$$

GOOD QUANTUM NUMBERS n, ℓ, s, m_ℓ, m_s

$$\boxed{H'_Z = \frac{e}{2m} B_{ext} \left(L_z + 2S_z \right)}$$

CHOOSE z-AXIS ALONG $\overline{B}_{ext}$.

↳ $$E'_{n\ell m_\ell m_s} = \langle n\ell m_\ell m_s \,|\, H'_Z \,|\, n\ell m_\ell m_s \rangle$$

$$\boxed{E'_{n\ell m_\ell m_s} = \mu_B B_{ext} \left(m_\ell + 2m_s \right)}$$

↳ H'_{FS} TREATED AS PERTURBATION.

$$H'_{SO} = \frac{1}{2} \alpha \frac{\hbar}{c} \frac{1}{m^2 r^3} \overline{L} \cdot \overline{S}$$

6.50

REPLACE

$$\langle \bar{L} . \bar{S} \rangle \simeq \underset{\underset{0}{\parallel}}{\langle L_x \rangle} \underset{\underset{0}{\parallel}}{\langle S_x \rangle} + \underset{\underset{0}{\parallel}}{\langle L_y \rangle} \underset{\underset{0}{\parallel}}{\langle S_y \rangle} + \langle L_z \rangle \langle S_z \rangle$$

$$= \hbar^2 m_\ell \, m_s .$$

$$E^1_{FS} = \frac{E_n^2}{2mc^2} \left\{ \underbrace{3 - \frac{4n}{\ell + \frac{1}{2}}}_{\text{REL. CORR.}} + \frac{4n \, m_\ell \, m_s}{\ell(\ell+\frac{1}{2})(\ell+1)} \right\}$$

$$\boxed{E^1_{FS} = \frac{(13.6)\, eV}{n^3} \left\{ \frac{3}{4n} - \frac{\ell(\ell+1) - m_\ell \, m_s}{\ell(\ell+\frac{1}{2})(\ell+1)} \right\}}$$

FINE-STRUCTURE CORR.

IN CASE OF STRONG EXT. FIELD

• INTERMEDIATE FIELD ZEEMAN EFFECT

WHEN $B_{int} \simeq B_{ext}$

TREAT H'_{FS} & H'_Z ON EQUAL FOOTING

↳ APPLY <u>DEGENERATE</u> PERTURBATION THEORY

IN UNPERTURBED BASIS $| n \ell j m_j \rangle$

$$W_{ij} = \langle \psi_i^0 | H'_{FS} + H'_Z | \psi_j^0 \rangle$$

$$|\psi_i^0\rangle = | n \ell j m_j \rangle$$

↳ $\langle n \ell j m_j | H'_{FS} | n' \ell' j' m_j' \rangle$

$$= \delta_{nn'} \delta_{\ell\ell'} \delta_{jj'} \delta_{m_j m_j'} \frac{E_n^2}{2mc^2} \left\{ 3 - \frac{4n}{j + \frac{1}{2}} \right\}$$

(WAS DONE ABOVE) ↳ DIAGONAL

↳ $\langle n \ell j m_j | H'_Z | n' \ell' j' m_j' \rangle$

$$= \frac{e}{2m} B_{ext} \langle n \ell j m_j | L_z + 2S_z | n \ell j m_j \rangle$$

EXPRESS

$$| n \ell j m_j \rangle = \sum_{m_\ell m_s} \overbrace{\langle \ell m_\ell, \tfrac{1}{2} m_s | j m_j \rangle}^{\text{CLEBSCH-GORDON COEFF.}} | n \ell m_\ell \rangle | \tfrac{1}{2} m_s \rangle$$

$\hookrightarrow$ EXAMPLE $\quad n = 2 \Rightarrow$ DEGENERACY $2n^2 = 8$

$$\quad\quad\quad |j\ m_j\rangle \quad\quad |\ell\ m_\ell\rangle \quad |\tfrac{1}{2}\ m_s\rangle$$

$\boxed{\ell = 0}$

$$\psi_1^0 \equiv |\tfrac{1}{2}\ {+\tfrac{1}{2}}\rangle = |0\ 0\rangle\ |\tfrac{1}{2}\ {+\tfrac{1}{2}}\rangle$$

$$\psi_2^0 \equiv |\tfrac{1}{2}\ {-\tfrac{1}{2}}\rangle = |0\ 0\rangle\ |\tfrac{1}{2}\ {-\tfrac{1}{2}}\rangle$$

$\boxed{\ell = 1}$

$$\psi_3^0 \equiv |\tfrac{3}{2}\ {+\tfrac{3}{2}}\rangle = |1\ 1\rangle\ |\tfrac{1}{2}\ {+\tfrac{1}{2}}\rangle$$

$$\psi_4^0 \equiv |\tfrac{3}{2}\ {-\tfrac{3}{2}}\rangle = |1\ {-1}\rangle\ |\tfrac{1}{2}\ {-\tfrac{1}{2}}\rangle$$

$$\psi_5^0 \equiv |\tfrac{3}{2}\ {+\tfrac{1}{2}}\rangle = \sqrt{\tfrac{2}{3}}\ |1\ 0\rangle\ |\tfrac{1}{2}\ {+\tfrac{1}{2}}\rangle + \sqrt{\tfrac{1}{3}}\ |1\ {+1}\rangle\ |\tfrac{1}{2}\ {-\tfrac{1}{2}}\rangle$$

$$\psi_7^0 \equiv |\tfrac{3}{2}\ {-\tfrac{1}{2}}\rangle = \sqrt{\tfrac{2}{3}}\ |1\ 0\rangle\ |\tfrac{1}{2}\ {-\tfrac{1}{2}}\rangle + \sqrt{\tfrac{1}{3}}\ |1\ {-1}\rangle\ |\tfrac{1}{2}\ {+\tfrac{1}{2}}\rangle$$

$$\psi_6^0 \equiv |\tfrac{1}{2}\ {+\tfrac{1}{2}}\rangle = -\sqrt{\tfrac{1}{3}}\ |1\ 0\rangle\ |\tfrac{1}{2}\ {+\tfrac{1}{2}}\rangle + \sqrt{\tfrac{2}{3}}\ |1\ {+1}\rangle\ |\tfrac{1}{2}\ {-\tfrac{1}{2}}\rangle$$

$$\psi_8^0 \equiv |\tfrac{1}{2}\ {-\tfrac{1}{2}}\rangle = \sqrt{\tfrac{1}{3}}\ |1\ 0\rangle\ |\tfrac{1}{2}\ {-\tfrac{1}{2}}\rangle - \sqrt{\tfrac{2}{3}}\ |1\ {-1}\rangle\ |\tfrac{1}{2}\ {+\tfrac{1}{2}}\rangle$$

$\hookrightarrow \langle \psi_1^0 | L_z + 2S_z | \psi_1^0 \rangle = +\hbar$

$\langle \psi_2^0 | L_z + 2S_z | \psi_2^0 \rangle = -\hbar$

NON-DIAGONAL ME INVOLVING 1 & 2 $\to 0$

$\hookrightarrow \langle \psi_3^0 | L_z + 2S_z | \psi_3^0 \rangle = \hbar (1 + 1) = 2\hbar$

$\langle \psi_4^0 | L_z + 2S_z | \psi_4^0 \rangle = \hbar (-1 - 1) = -2\hbar$

$\langle \psi_5^0 | L_z + 2S_z | \psi_5^0 \rangle = \hbar \left\{ \frac{2}{3} (0 + 1) + \frac{1}{3}(1-1) \right\}$

$= \hbar \frac{2}{3}$

$\langle \psi_6^0 | L_z + 2S_z | \psi_6^0 \rangle = \hbar \left\{ \frac{1}{3} (0 + 1) + \frac{2}{3}(1-1) \right\}$

$= \hbar \frac{1}{3}$

$\langle \psi_7^0 | L_z + 2S_z | \psi_7^0 \rangle = -\hbar \frac{2}{3}$

$\langle \psi_8^0 | L_z + 2S_z | \psi_8^0 \rangle = -\hbar \frac{1}{3}$

NON-DIAG. : ONLY BETWEEN ψ_5^0 & ψ_6^0

ψ_7^0 & ψ_8^0

ARE NON-ZERO

$\langle \psi_5^0 | L_z + 2S_z | \psi_6^0 \rangle = \hbar \left\{ -\frac{\sqrt{2}}{3} (0 + 1) + \frac{\sqrt{2}}{3}(1-1) \right\}$

$= -\hbar \frac{\sqrt{2}}{3}$

$\langle \psi_7^0 | L_z + 2S_z | \psi_8^0 \rangle = \hbar \left\{ \frac{\sqrt{2}}{3} (0 - 1) - \frac{\sqrt{2}}{3}(-1+1) \right\} = -\hbar \frac{\sqrt{2}}{3}$

$$\hookrightarrow \quad \underline{\underline{\beta \equiv \mu_B B_{ext}}} = \left(\frac{e\hbar}{2m}\right) B_{ext}$$

$$\hookrightarrow \quad \langle \underset{\substack{\uparrow \\ n}}{2} \; \underset{\substack{\uparrow \\ \ell}}{1} \; j \; m_j \,|\, H'_{FS} \,|\, 2 \; 1 \; j \; m_j \rangle$$

$$= \frac{(13.6\,eV)}{2^4} \frac{\frac{1}{2} mc^2 \alpha^2}{2mc^2} \left\{ 3 - \frac{8}{j+\frac{1}{2}} \right\}$$

$$= \underbrace{\left(\frac{\alpha}{8}\right)^2 (13.6\,eV)}_{\equiv \; \gamma} \cdot \underbrace{\left\{ 3 - \frac{8}{j+\frac{1}{2}} \right\}}$$

$j = \frac{3}{2}$: -1 $\qquad$ $j = \frac{1}{2}$: -5

$$W = -\begin{bmatrix} 5\gamma-\beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5\gamma+\beta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \gamma-2\beta & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma+2\beta & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \gamma-\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{3}\beta & 5\gamma-\frac{1}{3}\beta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \gamma+\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{3}\beta & 5\gamma+\frac{1}{3}\beta \end{bmatrix}$$

$\downarrow$

DIAGONALIZE W

- 4 EIGENVALUES
$$E_1' = -(5\gamma - \beta)$$
$$E_2' = -(5\gamma + \beta)$$
$$E_3' = -(\gamma - 2\beta)$$
$$E_4' = -(\gamma + 2\beta)$$

- DIAGONALIZE TWO 2×2 MATRICES.

$$\begin{vmatrix} \gamma - \frac{2}{3}\beta + \lambda & \frac{\sqrt{2}}{3}\beta \\ \frac{\sqrt{2}}{3}\beta & 5\gamma - \frac{1}{3}\beta + \lambda \end{vmatrix} = 0$$

$$\lambda^2 + (6\gamma - \beta)\lambda + \left(5\gamma^2 - \frac{11}{3}\beta\gamma\right) = 0$$

$$E_{5,6}' = \left(\frac{\beta}{2} - 3\gamma\right) \pm \sqrt{4\gamma^2 + \frac{2}{3}\beta\gamma + \frac{\beta^2}{4}}$$

- $$\begin{vmatrix} \gamma + \frac{2}{3}\beta + \lambda & \frac{\sqrt{2}}{3}\beta \\ \frac{\sqrt{2}}{3}\beta & 5\gamma + \frac{1}{3}\beta + \lambda \end{vmatrix} = 0$$

$$\lambda^2 + (6\gamma + \beta)\lambda + \left(5\gamma^2 + \frac{11}{3}\beta\gamma\right) = 0$$

$$E_{7,8}' = \left(-\frac{\beta}{2} - 3\gamma\right) \pm \sqrt{4\gamma^2 - \frac{2}{3}\beta\gamma + \frac{\beta^2}{4}}$$

↳ SPECIAL CASES

- $\underline{\beta = 0}$: NO EXTERNAL FIELD

$$E_1' = E_2' = E_6' = E_8' = -5\gamma \qquad (j = \tfrac{1}{2})$$
$$E_3' = E_4' = E_5' = E_7' = -\gamma \qquad (j = \tfrac{3}{2})$$
$$\Downarrow$$

RESULTS FROM H'_{FS}

- $\underline{\beta \ll \gamma}$ WEAK EXTERNAL FIELDS

$$E_1' = -5\gamma + \beta$$
$$E_2' = -5\gamma - \beta$$
$$E_3' = -\gamma + 2\beta$$
$$E_4' = -\gamma - 2\beta$$
$$E_5' = -\gamma + \tfrac{2}{3}\beta$$
$$E_6' = -5\gamma + \tfrac{1}{3}\beta$$
$$E_7' = -\gamma - \tfrac{2}{3}\beta$$
$$E_8' = -5\gamma - \tfrac{1}{3}\beta$$

NOTE: $\sqrt{4\gamma^2 + \frac{2}{3}\beta\gamma + \frac{\beta^2}{4}} \simeq 2\gamma\left(1 + \frac{\beta}{12\gamma}\right) = 2\gamma + \frac{\beta}{6}$

$\rightsquigarrow g_J = \frac{2}{3}$

↳ FIND BACK RESULTS OF WEAK FIELD ZEEMAN EFFECT

- $\underline{\beta \gg \gamma}$ → FIND BACK RESULTS OF STRONG FIELD ZEEMAN EFFECT

- $\underline{\underline{\beta \gg \gamma}}$ STRONG EXTERNAL FIELDS

$$E_1' = -5\gamma + \beta$$

$$E_2' = -5\gamma - \beta$$

$$E_3' = -\gamma + 2\beta$$

$$E_4' = -\gamma - 2\beta.$$

$$E_5' \cong \frac{\beta}{2} - 3\gamma + \frac{\beta}{2} \underbrace{\sqrt{1 + \frac{8}{3}\frac{\gamma}{\beta}}}_{\simeq 1 + \frac{4}{3}\frac{\gamma}{\beta}}$$

$$= \beta - \frac{7}{3}\gamma$$

$$E_6' \simeq \frac{\beta}{2} - 3\gamma - \frac{\beta}{2}\left(1 + \frac{4}{3}\frac{\gamma}{\beta}\right)$$

$$\simeq 0 - \frac{11}{3}\gamma$$

$$E_7' \simeq -\frac{\beta}{2} - 3\gamma + \frac{\beta}{2}\left(1 - \frac{4}{3}\frac{\gamma}{\beta}\right)$$

$$\simeq 0 - \frac{11}{3}\gamma$$

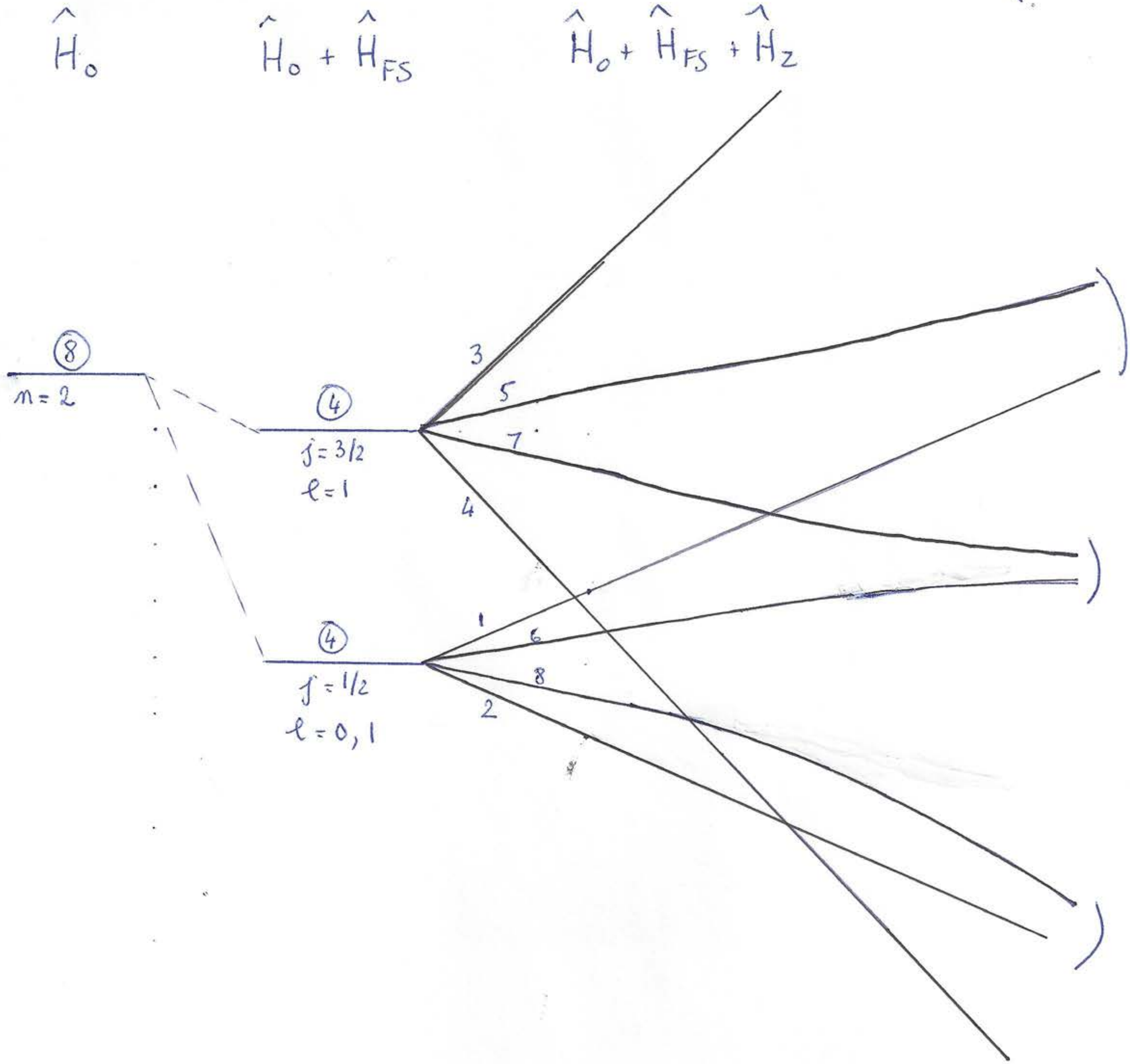
$$E_8' \simeq -\beta - \frac{7}{3}\gamma$$

FOR $\beta \gg \gamma$ (5 LEVELS)

$$E_1' = E_5' = \beta \qquad E_3' = 2\beta \qquad E_6' = E_7' = 0$$

$$E_2' = E_8' = -\beta \qquad E_4' = -2\beta$$

6.56 c


$\hat{H}_0$
$\hat{H}_0 + \hat{H}_{FS}$
$\hat{H}_0 + \hat{H}_{FS} + \hat{H}_Z$
8
$n = 2$
4
$j = 3/2$
$\ell = 1$
4
$j = 1/2$
$\ell = 0, 1$
3
5
7
4
1
6
8
2

$\Rightarrow$ HYPERFINE SPLITTING IN H

- ZERO RANGE INTERACTION BETWEEN 2 MAGNETIC DIPOLE MOMENTS $\bar{\mu}_1$ & $\bar{\mu}_2$

$$\hat{H} = -\frac{2}{3}\mu_0 \; \bar{\mu}_1 \cdot \bar{\mu}_2 \; \delta^3(\bar{r})$$

(see E&M : MAGNETOSTATICS)

- SPIN-SPIN INTERACTION BETWEEN e^- SPIN & PROTON SPIN IN HYDROGEN

$$\bar{\mu}_e = -\, g_e \frac{e}{2m_e} \bar{S}_e \quad , \quad g_e = 2$$

$$\bar{\mu}_p = +\, g_p \frac{e}{2m_p} \bar{S}_p \quad , \quad g_p = 5.59$$

<u>NOTE</u> $m_e \simeq 0.511$ MeV

$m_p \simeq 938.3$ MeV

$$\frac{m_e}{m_p} \simeq \frac{1}{2000}$$

$$\boxed{\hat{H}_{HF} = +\frac{1}{3}\mu_0 \frac{e^2 g_P}{m_e m_p} \bar{S}_e \cdot \bar{S}_p \, \delta^3(\bar{r})}$$

HYPERFINE
INTERACTION
IN $\ell = 0$ STATE OF HYDROGEN

SPIN-SPIN
INTERACTION

- $\bar{S}_e \cdot \bar{S}_p = \frac{1}{2}\left(S^2 - S_e^2 - S_p^2\right)$

$\uparrow_p \quad \uparrow_{e^-} \quad S = 1 \quad \Rightarrow \langle \bar{S}_e \cdot \bar{S}_p \rangle = \frac{\hbar^2}{2} \cdot \left(2 - \frac{3}{2}\right) = \frac{\hbar^2}{4}$

$\uparrow_p \quad \downarrow e^- \quad S = 0 \quad \Rightarrow \langle \bar{S}_e \cdot \bar{S}_p \rangle = \frac{\hbar^2}{2}\left(-\frac{3}{2}\right) = -\frac{3\hbar^2}{4}$

- $\langle \delta^3(\bar{r}) \rangle = \frac{1}{\pi a^3} = |\psi_{100}(0)|^2$ FOR $\underline{\underline{n = 1, \ \ell = 0}}$

- $$\boxed{E^1_{HF}(n=1, \ell=0) = \frac{\mu_0}{3} \frac{e^2 g_P}{\pi a^3 m_e m_p} \cdot \hbar^2 \cdot \begin{cases} +\frac{1}{4} & (S=1) \\ -\frac{3}{4} & (S=0) \end{cases}}$$

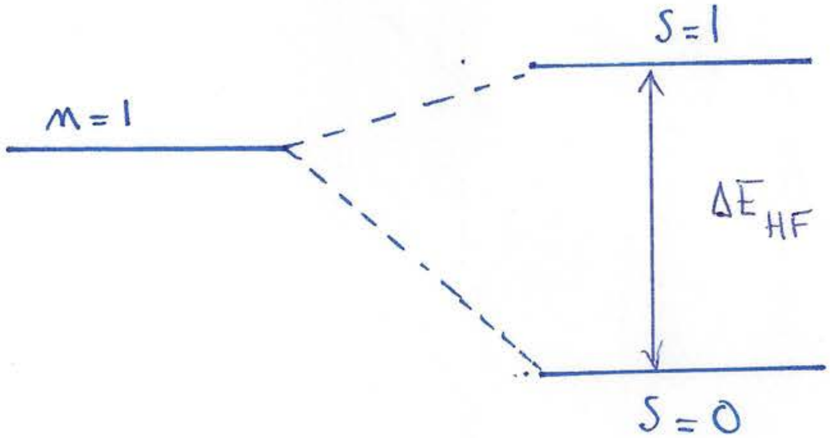
$$\rightsquigarrow \mu_0 \frac{e^2}{\pi} = \frac{e^2}{\pi \varepsilon_0 c^2} = 4\alpha \frac{\hbar}{c} \qquad \left(\alpha = \frac{1}{137}\right)$$

$$\rightsquigarrow a = \frac{1}{m_e \alpha} \frac{\hbar}{c} \qquad \rightsquigarrow -E_1 = \alpha^2 \frac{1}{2} m_e c^2$$

$$\frac{1}{a^3} = m_e^3 \alpha^3 \frac{c^3}{\hbar^3}$$

$$\rightsquigarrow E^1_{HF}(n=1, \ell=0) = \frac{4}{3} \alpha^4 g_p \frac{m_e^2 c^2}{m_p} \cdot \begin{cases} 1/4 & (S=1) \\ -3/4 & (S=0) \end{cases}$$

$$= \underbrace{(-E_1)}_{13.6\,eV} \cdot \underbrace{\alpha^2 \frac{m_e}{m_p}}_{\sim 10^{-4} \; \sim 10^{-3}} \frac{8}{3} g_p \begin{cases} 1/4 & (S=1) \\ -3/4 & (S=0) \end{cases}$$



$$\boxed{\Delta E_{HF} = (-E_1) \cdot \alpha^2 \frac{m_e}{m_p} \frac{8}{3} g_p}$$

$$\underline{\underline{\Delta E_{HF} \simeq 5.88\ 10^{-6}\ eV}}$$

$$\Delta E_{HF} = h\nu$$

$$= \frac{hc}{\lambda}$$

$$\lambda = \frac{\hbar c\ 2\pi}{\Delta E_{HF}} = \frac{(197\ eV\ 10^{-9} m)\ 2\pi}{5.88\ 10^{-6}\ eV}$$

$$\simeq 21\ 10^{-2}\ m$$

$$\underline{\boxed{\lambda = 21\ cm}}$$

$$\Downarrow$$

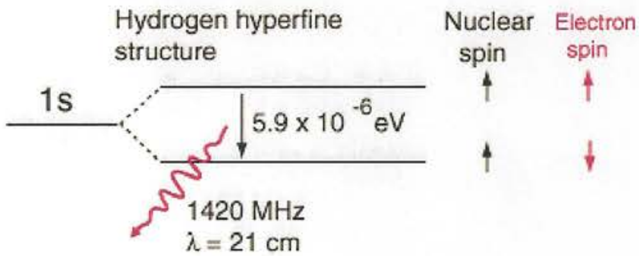
21 cm line IN RADIO ASTRONOMY !

EMITTED BY H-GAS IN INTERSTELLAR REGION

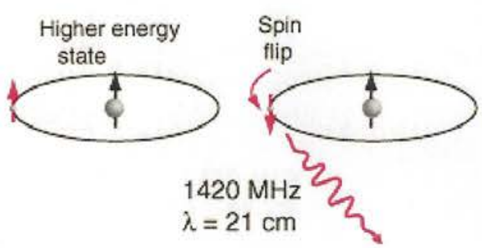
The Hydrogen 21-cm Line

The hydrogen in our galaxy has been mapped by the observation of the 21-cm wavelength line of hydrogen gas. At 1420 MHz, this radiation from hydrogen penetrates the dust clouds and gives us a more complete map of the hydrogen than that of the stars themselves since their visible light won't penetrate the dust clouds.

The 1420 MHz radiation comes from the transition between the two levels of the hydrogen 1s ground state, slightly split by the interaction between the electron spin and the nuclear spin. The splitting is known as hyperfine structure. Because of the quantum properties of of radiation, hydrogen in its lower state will absorb 1420 MHz and the observation of 1420 MHz in emission implies a prior excitation to the upper state.



This splitting of the hydrogen ground state is extremely small compared to the ground state energy of -13.6 eV, only about two parts in a million. The two states come from the fact that both the electron and nuclear spins are 1/2 for the proton, so there are two possible states, spin parallel and spin antiparallel. The state with the spins parallel is slightly higher in energy (less tightly bound).



In visualizing the transition as a spin-flip, it should be noted that the quantum mechanical property called "spin" is not literally a classical spinning charge sphere. It is a description of the behavior of quantum mechanical angular momentum and does not have a definitive classical analogy.

The observation of the 21cm line of hydrogen marked the birth of spectral-line radio astronomy. It was first observed in 1951 by Harold Ewen and Edward M. Purcell at Harvard, followed soon afterward by observers in Holland and Australia. The prediction that the 21 cm line should be observable in emission was made in 1944 by Dutch astronomer H. C. van de Hulst.

Index

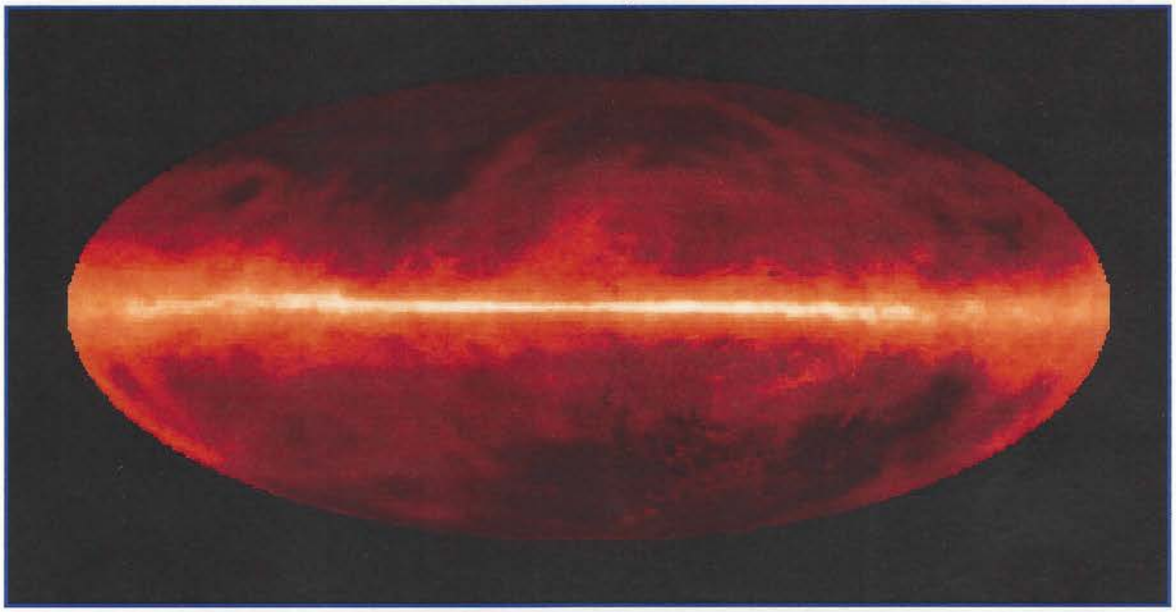
Hydrogen concepts

Reference Harwit.

Astronomy Picture of the Day

Discover the cosmos! Each day a different image or photograph of our fascinating universe is featured, along with a brief explanation written by a professional astronomer.

December 18, 1996



A Sky Full Of Hydrogen
Credit: J. Dickey (UMn), F. Lockman (NRAO), SkyView

Explanation: Interstellar space is filled with extremely tenuous clouds of gas which are mostly Hydrogen. The neutral hydrogen atom (HI in astronomer's shorthand) consists of 1 proton and 1 electron. The proton and electron spin like tops but can have only two orientations; spin axes parallel or anti-parallel. It is a rare event for Hydrogen atoms in the interstellar medium to switch from the parallel to the anti-parallel configuration, but when they do they emit radio waves with a wavelength of 21 centimeters (about 8 inches) and a corresponding frequency of exactly 1420 MHz. Tuned to this frequency radio telescopes have mapped the neutral Hydrogen in the sky. The above image represents such an all-sky HI survey with the plane of our Milky Way Galaxy running horizontally through the center. In this false color image no stars are visible, just diffuse clouds of gas tens to hundreds of light years across which cluster near the plane. The gas clouds seem to form arching, looping structures, stirred up by stellar activity in the galactic disk.

Tomorrow's picture: Comet Hale-Bopp Inbound

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