Charles Darwin (1887-1962)

Fine Structure

Willis Lamb (1913-2008)

Read McIntyre 12.1-12.2

PH451/551

PAM Dirac (1902-1984)

Reading Quiz

Numbers for

1. Ground state energy of H in eV: $E_{1s}^{(0)}$?
2. Mass of the electron in eV: m_e?
3. Fine structure constant: α?

Reading Quiz

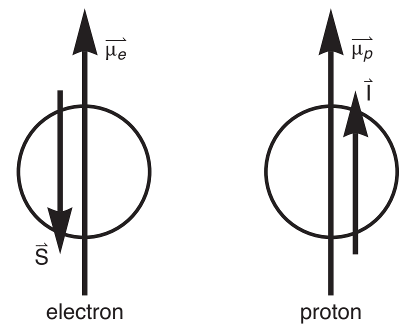
Numbers for

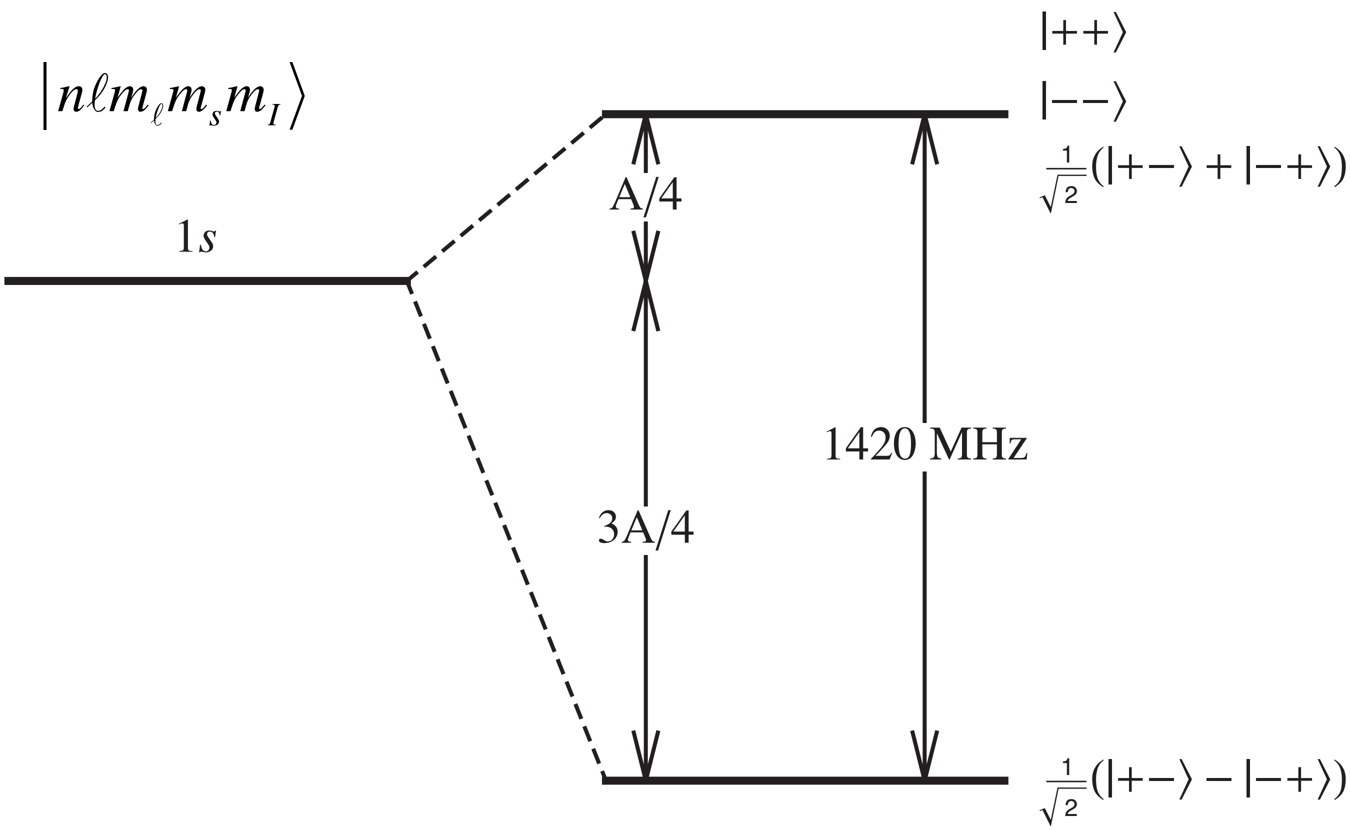
1. Ground state energy of H in eV: $E_{1s}^{(0)}$? -13.6 eV
2. Mass of the electron in eV: m_e? 0.511 MeV
3. Fine structure constant: α?

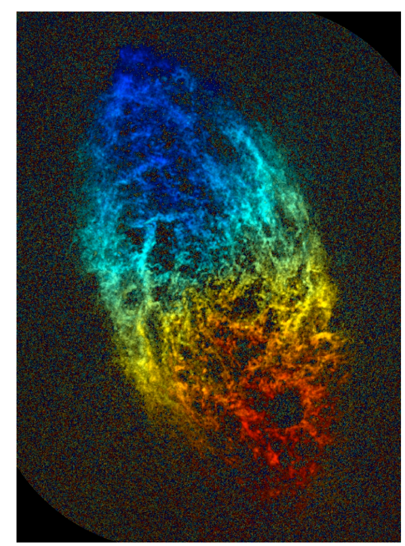
$$\alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c} = \frac{1}{137}$$

Recap: The hyperfine interaction lifts the degeneracy of the H ground state

1. Hyperfine interaction: $H'_{hf} = \frac{\mu_0}{4\pi}\frac{g_e\mu_B g_p\mu_N}{\hbar^2}\frac{8\pi}{3}\mathbf{S}\bullet\mathbf{I}\,\delta(\mathbf{r}) = \frac{A}{\hbar^2}\mathbf{S}\bullet\mathbf{I}$







Recap: C-G coefficients

1. See summary sheet for am relations:

$$\left|F, m_F\right\rangle \qquad \left|m_s m_I\right\rangle$$

$$\left|F, m_F = F\right\rangle = \left|++\right\rangle$$

$$\left|F, m_F = -F\right\rangle = \left|--\right\rangle$$

$s=\frac{1}{2}$, $I=\frac{1}{2}$		F	1	1	1	0
		M_F	1	0	−1	0
m_s	m_I					
$\frac{1}{2}$	$\frac{1}{2}$		1	0	0	0
$\frac{1}{2}$	$-\frac{1}{2}$		0	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$
$-\frac{1}{2}$	$\frac{1}{2}$		0	$\frac{1}{\sqrt{2}}$	0	$-\frac{1}{\sqrt{2}}$
$-\frac{1}{2}$	$-\frac{1}{2}$		0	0	1	0

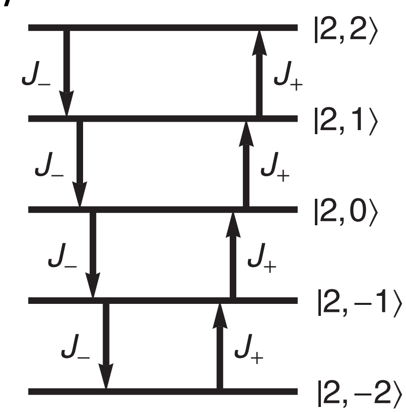
$$J_{\pm}\left|j, m_j\right\rangle = \hbar\left[j(j+1) - m_j(m_j \pm 1)\right]^{1/2}\left|j, m_j \pm 1\right\rangle$$

$$J_+ = \left(J_x + iJ_y\right)$$

$$J_- = \left(J_x - iJ_y\right)$$

$$\left[J_+, J_-\right] = 2\hbar J_z$$

$$J_+\left|j, j\right\rangle = 0; \quad J_-\left|j, -j\right\rangle = 0$$



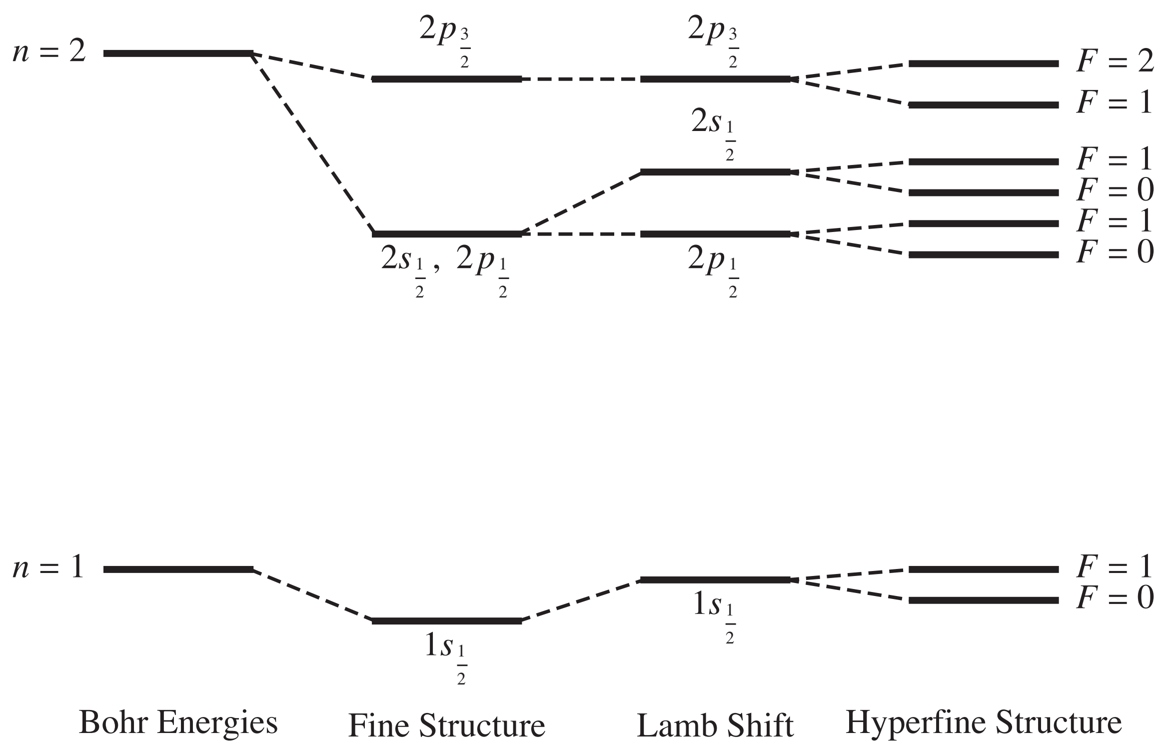
Fine Structure

forget about proton spin now-that's hyperfine!

1. Scale:

Table 12.1: Hydrogen energy scales

Term	Scale
Bohr energy	$\alpha^2 mc^2$
Fine structure	$\alpha^4 mc^2$
Lamb shift	$\alpha^5 mc^2$
Hyperfine structure	$(m_e/m_p)\alpha^4 mc^2$



2. Fine structure:
   - relativistic speed of electron
   - spin-orbit coupling
   - (Lamb shift; s-states only)

Relativistic correction DOWNWARD

1. (Almost) Straightforward application of perturbation theory (PT)
2. Why can we use "non-degenerate" PT for this part?
3. Results (do for HW):

$$E = mc^2\sqrt{1+\left(\frac{p}{mc}\right)^2} \Rightarrow H'_{rel} = -\frac{p^4}{8m^4c^2}$$

$$\left\langle \frac{1}{r} \right\rangle_{n\ell} = \int_0^\infty \frac{1}{r} R_{n\ell}^2(r) r^2\, dr = \frac{1}{n^2 a_0}$$

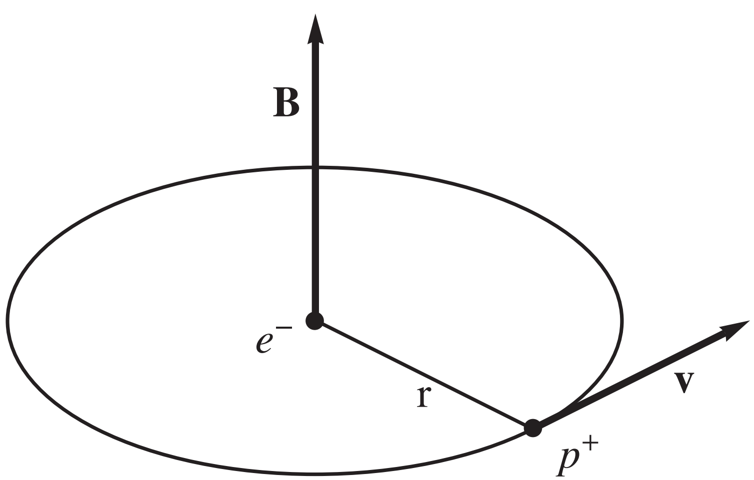
$$\left\langle \frac{1}{r^2} \right\rangle_{n\ell} = \int_0^\infty \frac{1}{r^2} R_{n\ell}^2(r) r^2\, dr = \frac{1}{\left(\ell+\frac{1}{2}\right) n^3 a_0^2}$$

$$E_{rel}^{(1)} = -\frac{1}{2}\alpha^4 mc^2 \left[\frac{1}{n^3\left(\ell+\frac{1}{2}\right)} - \frac{3}{4n^4}\right]$$

Spin-orbit correction:

Simple application of angular momentum addition

1. Electron ORBITAL magnetic moment and SPIN magnetic moment interact!



$$\mathbf{B} = \frac{e}{4\pi\varepsilon_0 mc^2 r^3}\mathbf{L}$$

$$B = \frac{e}{4\pi\varepsilon_0 m \underbrace{c^2}_{\frac{1}{\varepsilon_0\mu_0}} r r^2} \underbrace{L}_{m\omega r^2}$$

$$B = \mu_0 \frac{e \overbrace{\omega}^{2\pi/T}}{4\pi r}$$

$$B = \mu_0 \frac{I}{2r} \quad \text{(B-S law)}$$

Spin-orbit correction:

Simple application of angular momentum addition

1. Electron ORBITAL magnetic moment and SPIN magnetic moment interact.

$$H'_{so} = -\left(-\frac{e}{m}\mathbf{S}\right)\bullet\frac{e}{4\pi\varepsilon_0 mc^2 r^3}\mathbf{L}$$

$$= \frac{e^2}{4\pi\varepsilon_0 m^2c^2r^3}\mathbf{L}\bullet\mathbf{S}$$

$$H'_{so} = \frac{e^2}{4\pi\varepsilon_0 m^2c^2r^3}\tfrac{1}{2}\left(\mathbf{J}^2-\mathbf{L}^2-\mathbf{S}^2\right)$$

2. Total am

$$\mathbf{J} = \mathbf{L}+\mathbf{S}$$

$$\mathbf{J}^2 = \mathbf{L}^2+\mathbf{S}^2+2\mathbf{L}\bullet\mathbf{S}$$

$$\mathbf{L}\bullet\mathbf{S} = \tfrac{1}{2}\left(\mathbf{J}^2-\mathbf{L}^2-\mathbf{S}^2\right)$$

3. Coupled, uncoupled states?

Spin-orbit correction:

Simple application of angular momentum addition

1. Coupled states give diagonal basis for H'_{SO}

$$J^2\left| j, m_j \ell s \right\rangle = ?$$

$$L^2\left| j, m_j \ell s \right\rangle = ?$$

$$S^2\left| j, m_j \ell s \right\rangle = ?$$

2. How do generate coupled states from uncoupled states that we already know? CG coefficients!

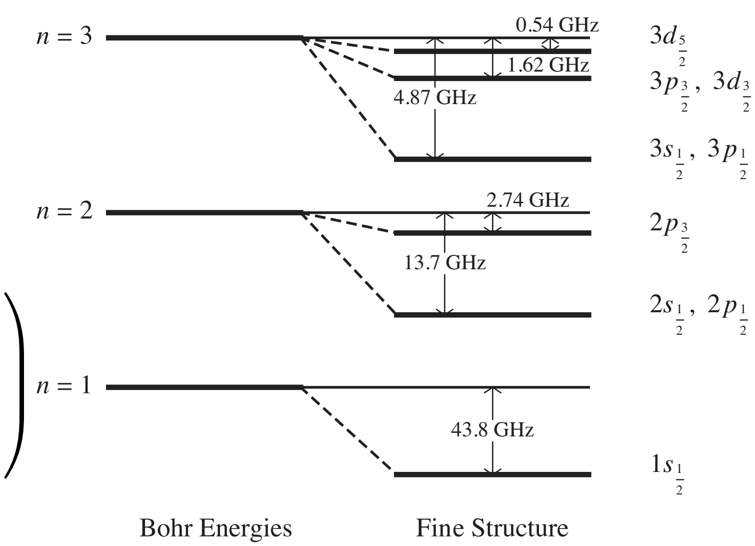
Spin-orbit correction:

Ground state *n*=1; no correction *L*=0!

1. n=1 uncoupled

$$\left|\ell m_\ell s m_s\right\rangle_u : \quad \left|0,0,\tfrac{1}{2},\tfrac{1}{2}\right\rangle_u ; \quad \left|0,0,\tfrac{1}{2},-\tfrac{1}{2}\right\rangle_u$$

$$\left|\ell m_\ell s m_s\right\rangle_u \doteq Y_{00}(\theta,\phi)\begin{pmatrix}1\\0\end{pmatrix}; Y_{00}(\theta,\phi)\begin{pmatrix}0\\1\end{pmatrix}$$



2. n=1 coupled states:

$$\left|J m_J \ell s\right\rangle_c : \left|\tfrac{1}{2},\tfrac{1}{2},\cancel{0},\cancel{\tfrac{1}{2}}\right\rangle_c ; \left|\tfrac{1}{2},-\tfrac{1}{2},\cancel{0},\cancel{\tfrac{1}{2}}\right\rangle_c$$

$$\left|J m_J \cancel{\ell s}\right\rangle : \ {}^{2S+1}L_J = {}^2S_{1/2}$$

coupled= $\sum$ uncoupled

$$\left|\tfrac{1}{2},\tfrac{1}{2}\,\cancel{0,\tfrac{1}{2}}\right\rangle_c = \left|0,0,\tfrac{1}{2},\tfrac{1}{2}\right\rangle_u$$

$$\left|\tfrac{1}{2},-\tfrac{1}{2},\cancel{0,\tfrac{1}{2}}\right\rangle_c = \left|0,0,\tfrac{1}{2},-\tfrac{1}{2}\right\rangle_u$$

Both stretched states, so

Spin-orbit correction: general

1. E_{SO} ? Diagonalize the S-O perturbationHamiltonian in the degenerate subspace ….

$$H'_{SO} = \frac{e^2}{4\pi\varepsilon_0 m^2 c^2 r^3}\tfrac{1}{2}\left(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2\right)$$

$$\begin{aligned} E_{SO} &= {}_c\langle j m_j \ell s | H'_{SO} | j m_j \ell s \rangle_c \\ &= \frac{e^2}{4\pi\varepsilon_0 m^2 c^2}\, {}_c\left\langle j m_j \ell s \right| \frac{1}{r^3}\frac{1}{2}\left(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2\right) \left| j m_j \ell s \right\rangle_c \end{aligned}$$

$$E_{SO}^{(1)} = \frac{e^2}{4\pi\varepsilon_0 m^2 c^2} \underbrace{\left\langle \frac{1}{r^3} \right\rangle}_{\frac{1}{a_0^3 n^3 \ell\left(\ell+\frac{1}{2}\right)\left(\ell+1\right)}} \tfrac{1}{2}\Big(j\left(j+1\right) - \ell\left(\ell+1\right) - s\left(s+1\right)\Big)\hbar^2$$

Spin-orbit correction: *n*=1

1. E_{SO} (*n* = 1): *l* = 0 so SOC is **L•S** = 0!

$$H'_{SO} = \frac{e^2}{4\pi\varepsilon_0 m^2 c^2 r^3} \tfrac{1}{2}\left(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2\right)$$

$$E_{SO} = \frac{e^2}{4\pi\varepsilon_0 m^2 c^2} \underbrace{\left\langle \frac{1}{r^3} \right\rangle}_{\frac{1}{a_0^3 n^3 \ell\left(\ell+\frac{1}{2}\right)\left(\ell+1\right)}} \tfrac{1}{2}\underbrace{\left(\left(\tfrac{1}{2}\cdot\tfrac{3}{2}\right)^2 - \left(0\cdot 0\right)^2 - \left(\tfrac{1}{2}\cdot\tfrac{3}{2}\right)^2\right)}_{=0}$$

2. Notice 0/0 ….? The *l* = 0 problem is discussed in the book – it is the so-called Darwin term. Upshot is that it is taken care of when we write states in terms of *J*, not *l* and *s*.

Spin-orbit correction: (*n*=2, *l*=0)

1. *n*=2, *l*=0 uncoupled states

$$\left|\ell m_\ell s m_s\right\rangle_u : \left|0,0,\tfrac{1}{2},\tfrac{1}{2}\right\rangle_u ; \left|0,0,\tfrac{1}{2},-\tfrac{1}{2}\right\rangle_u$$

$$\left|\ell m_\ell s m_s\right\rangle_u \doteq Y_{00}(\theta,\phi)\begin{pmatrix} 1 \\ 0 \end{pmatrix} ; Y_{00}(\theta,\phi)\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

2. Coupled states are the same

3. E_{SO} = 0 as before for *n*=1, *l*=0

Spin-orbit correction: (n=2, l=1)

1. n=2, l=1 (2p) uncoupled states

$$\left|\ell m_\ell s m_s\right\rangle_u :$$

$$\left|1,1,\tfrac{1}{2},\tfrac{1}{2}\right\rangle_u ; \left|1,1,\tfrac{1}{2},-\tfrac{1}{2}\right\rangle_u ; \left|1,0,\tfrac{1}{2},\tfrac{1}{2}\right\rangle_u ; \left|1,0,\tfrac{1}{2},-\tfrac{1}{2}\right\rangle_u ; \left|1,-1,\tfrac{1}{2},\tfrac{1}{2}\right\rangle_u ; \left|1,-1,\tfrac{1}{2},-\tfrac{1}{2}\right\rangle_u$$

$$\left|\ell m_\ell s m_s\right\rangle_u \doteq \underbrace{Y_{1m_\ell}(\theta,\phi)\begin{pmatrix}1\\0\end{pmatrix}}_{\text{3 of these}} ; \underbrace{Y_{1m_\ell}(\theta,\phi)\begin{pmatrix}0\\1\end{pmatrix}}_{\text{3 of these}}$$

Spin-orbit correction: (n=2, l=1)

1. n=2 , J=3/2 and J=½ states) coupled states:

$$\left|Jm_J\ell s\right\rangle_c : \left|\tfrac{1}{2},\pm\tfrac{1}{2},1,\tfrac{1}{2}\right\rangle_c; \quad {}^2P_{1/2} \quad \left({}^{2S+1}L_J\right)$$

$$\left|Jm_J\ell s\right\rangle_c : \left|\tfrac{3}{2},\pm\tfrac{3}{2},1,\tfrac{1}{2}\right\rangle_c; \left|\tfrac{3}{2},\pm\tfrac{1}{2},1,\tfrac{1}{2}\right\rangle_c \quad {}^2P_{3/2} \quad \left({}^{2S+1}L_J\right)$$

2. TERM SYMBOL (just more notation …)

$$^{2S+1}L_J$$

Spin-orbit correction (states): (n=2, l=1)

3. Use C-G coefficients (HW) to write   coupled=$\sum$uncoupled

(a) Stretched ${}^2P_{3/2}$ state

$$\left| j=\tfrac{3}{2}, m_j\, \tfrac{3}{2}, \ell=1, s=\tfrac{1}{2}\right\rangle_c = \left| \ell=1, m_\ell=1, s=\tfrac{1}{2}, m_s=\tfrac{1}{2}\right\rangle_u$$

(b) Rest of ${}^2P_{3/2}$ states

$$\left|\tfrac{3}{2},\tfrac{1}{2},1,\tfrac{1}{2}\right\rangle_c = ?\left|\ell=1, m_\ell=1, s=\tfrac{1}{2}, m_s=\tfrac{1}{2}\right\rangle_u + ?\left|1,1,\tfrac{1}{2},\tfrac{-1}{2}\right\rangle_u + ?\left|1,0,\tfrac{1}{2},\tfrac{1}{2}\right\rangle_u$$
$$+ ?\left|1,0,\tfrac{1}{2},\tfrac{-1}{2}\right\rangle_u + ?\left|1,-1,\tfrac{1}{2},\tfrac{1}{2}\right\rangle_u + ?\left|1,-1,\tfrac{1}{2},\tfrac{-1}{2}\right\rangle_u$$

$$\left|\tfrac{3}{2},\tfrac{-1}{2},1,\tfrac{1}{2}\right\rangle_c = ?\left|1,1,\tfrac{1}{2},\tfrac{1}{2}\right\rangle_u + ?\left|1,1,\tfrac{1}{2},\tfrac{-1}{2}\right\rangle_u + ?\left|1,0,\tfrac{1}{2},\tfrac{1}{2}\right\rangle_u$$
$$+ ?\left|1,0,\tfrac{1}{2},\tfrac{-1}{2}\right\rangle_u + ?\left|1,-1,\tfrac{1}{2},\tfrac{1}{2}\right\rangle_u + ?\left|1,-1,\tfrac{1}{2},\tfrac{-1}{2}\right\rangle_u$$

$$\left|\tfrac{3}{2},\tfrac{-3}{2},1,\tfrac{1}{2}\right\rangle_c = ?\left|1,1,\tfrac{1}{2},\tfrac{1}{2}\right\rangle_u + ?\left|1,1,\tfrac{1}{2},\tfrac{-1}{2}\right\rangle_u + ?\left|1,0,\tfrac{1}{2},\tfrac{1}{2}\right\rangle_u$$
$$+ ?\left|1,0,\tfrac{1}{2},\tfrac{-1}{2}\right\rangle_u + ?\left|1,-1,\tfrac{1}{2},\tfrac{1}{2}\right\rangle_u + ?\left|1,-1,\tfrac{1}{2},\tfrac{-1}{2}\right\rangle_u$$

(c) ${}^2P_{1/2}$states?

Spin-orbit correction (energy): (*n*=2, *l*=1)

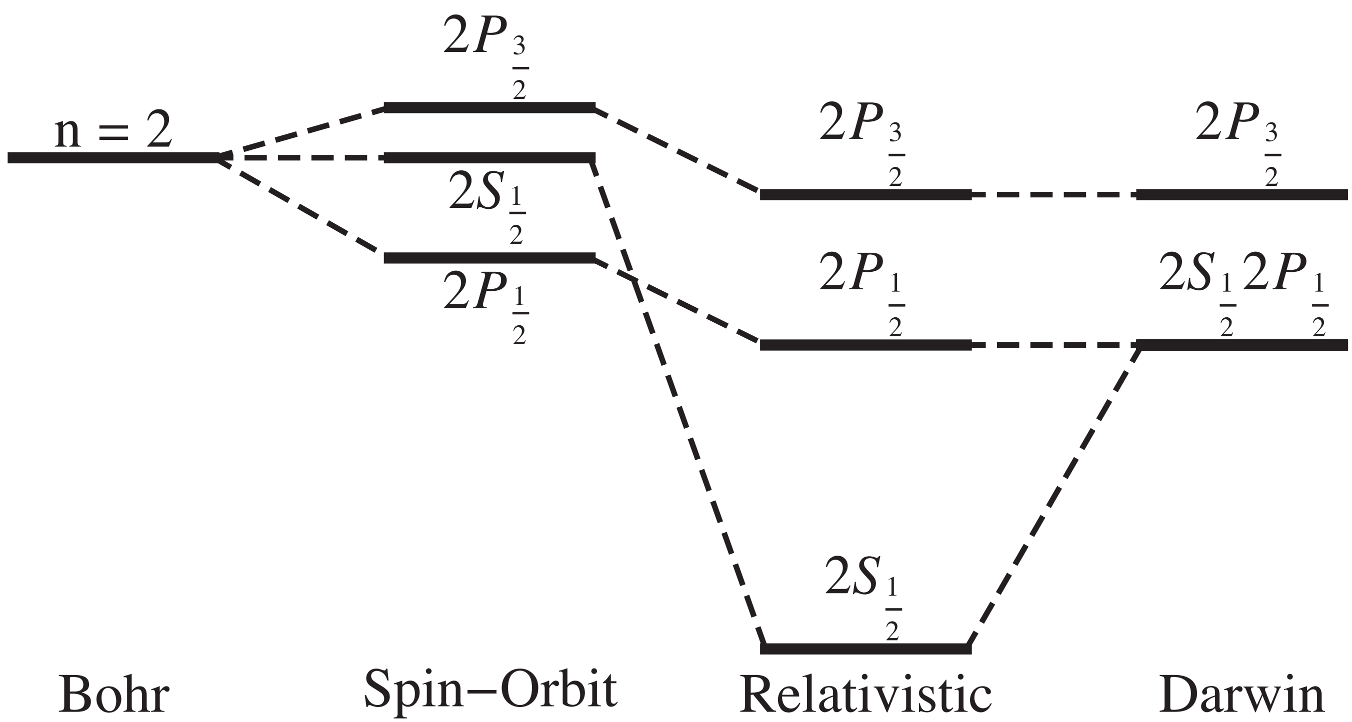
1. E_{SO} (n=2): in the *L*=1 subspace L•S≠0

$$H'_{SO} = \frac{e^2}{4\pi\varepsilon_0 m^2 c^2 r^3} \tfrac{1}{2}\left(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2\right)$$

$$E_{SO}^{(1)} = \frac{e^2}{4\pi\varepsilon_0 m^2 c^2} \underbrace{\left\langle \frac{1}{r^3} \right\rangle}_{\frac{1}{a_0^3 n^3 \ell\left(\ell+\frac{1}{2}\right)(\ell+1)\neq 0}} \underbrace{\tfrac{1}{2}\left(j(j+1) - \ell(\ell+1) - \tfrac{3}{4}\right)}_{\neq 0}\hbar^2$$

$$E_{SO}^{(1)} = \frac{1}{4}\alpha^4 mc^2 \frac{j(j+1) - \ell(\ell+1) - \frac{3}{4}}{n^3 \ell\left(\ell+\frac{1}{2}\right)(\ell+1)}$$

S-O and rel correction (UP or DOWN?)

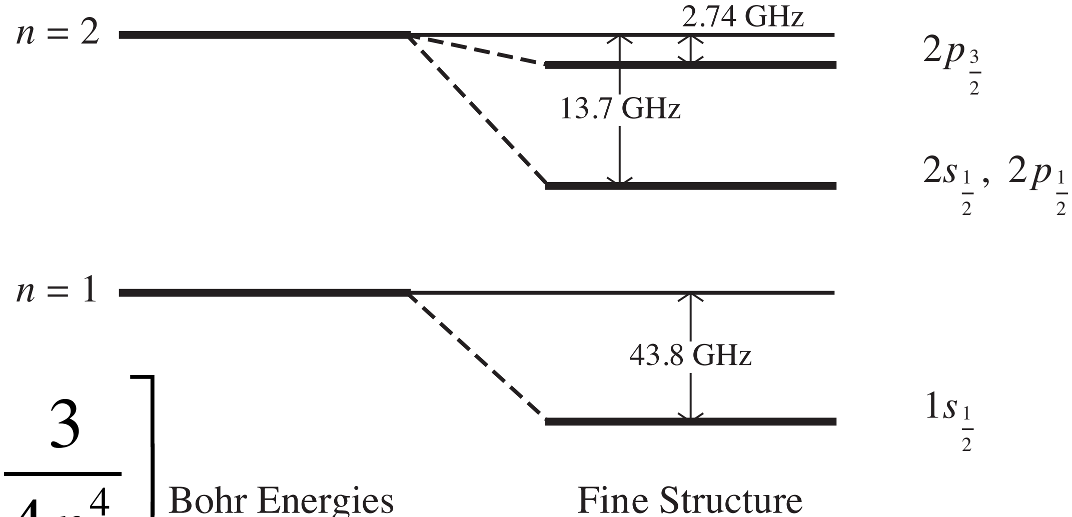


$$E_{rel}^{(1)} = -\frac{1}{2}\alpha^4 mc^2\left[\frac{1}{n^3\left(\ell+\frac{1}{2}\right)} - \frac{3}{4n^4}\right]$$

$$E_{SO}^{(1)} = \frac{1}{4}\alpha^4 mc^2\,\frac{j\left(j+1\right)-\ell\left(\ell+1\right)-\frac{3}{4}}{n^3\ell\left(\ell+\frac{1}{2}\right)\left(\ell+1\right)}$$

Fine structure correction

1. Put E_{SO} and E_{rel} together to get:



$$E_{rel}^{(1)} = -\frac{1}{2}\alpha^4 mc^2 \left[\frac{1}{n^3\left(\ell+\frac{1}{2}\right)} - \frac{3}{4n^4}\right]$$

$$E_{SO}^{(1)} = \frac{1}{4}\alpha^4 mc^2 \frac{j(j+1)-\ell(\ell+1)-\frac{3}{4}}{n^3\ell\left(\ell+\frac{1}{2}\right)(\ell+1)}$$

$$E_{fs}^{(1)} = E_{rel}^{(1)} + E_{SO}^{(1)} = -\frac{1}{2}\alpha^4 mc^2 \frac{1}{n^3}\left[\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right]$$