Phys 438/538, 1st Midterm Solutions 22 March 2013

1] Fine structure shift in H, 2s state. $Z=1$

* Starting with SOI: $\hat{\mathcal{H}}_{SO} = \lambda \vec{l}\cdot\vec{s}$. Since for 2s $l=0$, $\Delta E_{SO}=0$

* Relativistic mass correction: $\hat{\mathcal{H}}_R = -\frac{p^4}{8m_e^3c^2}$

$$= -\frac{1}{2m_ec^2}\left[H_0 - V\right]^2$$

$$\Delta E_R = -\frac{1}{2m_ec^2}\langle \underbrace{H_0^2}_{E_{2s}^2} + V^2 - 2H_0V\rangle_{2s}$$

$$\langle H_0 V\rangle_{2s} = -\frac{e^2}{4\pi\varepsilon_0}E_{2s}\left\langle\frac{1}{r}\right\rangle_{2s} = -\frac{e^2}{4\pi\varepsilon_0}\frac{E_{2s}}{4a_B}$$

we use supplied $\langle r^\gamma\rangle$ moments

$$\langle V^2\rangle_{2s} = \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\left\langle\frac{1}{r^2}\right\rangle_{2s} = \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\frac{1}{4a_B^2}$$

$$\Rightarrow \Delta E_R = \frac{-E_{2s}}{2m_ec^2}\left[E_{2s} + \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\frac{1}{4E_{2s}a_B^2} + \overbrace{2\frac{e^2}{4\pi\varepsilon_0}\frac{1}{4a_B}}^{-2H_0V}\right]$$

use: $\frac{e^2}{4\pi\varepsilon_0} = \alpha\hbar c$, $E_{2s} = -\frac{m_ec^2}{8}\alpha^2$

$$= \frac{\alpha^2}{16}\left[-\frac{m_ec^2\alpha^2}{8} + \alpha^2\hbar^2c^2\frac{-8}{m_ec^2\alpha^2}\cdot\frac{m_e^2c^2\alpha^2}{4\hbar^2} + 2\alpha\hbar c\frac{m_ec\alpha}{4\hbar}\right]$$

$$\Delta E_R = \frac{\alpha^2}{16}m_ec^2\left[-\frac{\alpha^2}{8} - 2\alpha^2 + \frac{\alpha^2}{2}\right] = -m_ec^2\alpha^4\frac{13}{128}$$

* Darwin term: $\hat{\mathcal{H}}_D = \dfrac{e^2\hbar^2}{8m_e^2c^2\varepsilon_0}\,\delta(\vec{r})$

$$\Delta E_D = \frac{e^2\hbar^2}{8m_e^2c^2\varepsilon_0}\underbrace{\left|\psi_{2s}(0)\right|^2}_{\frac{1}{8\pi a_B^3}} \qquad a_B = \frac{\hbar}{m_e c\alpha}$$

$$= m_e c^2\alpha^4\,\frac{1}{16}$$

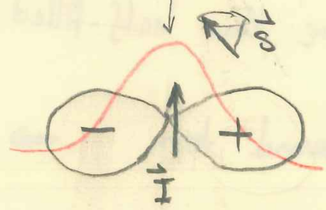
The total fine-structure shift becomes:

$$\Delta E_{FS}(2s) = m_e c^2\alpha^4\underbrace{\left(-\frac{13}{128}+\frac{1}{16}\right)}_{-\frac{5}{128}}$$

2] 1s state hyperfine shift for D

* Since $l=0$, the orbital contribution $(\vec{l}\cdot\vec{I})$ vanishes.

* Again for $l=0$ wf the dipolar part vanishes due to angular part of integration



OR do the integration (angular part) to believe

* So, only Fermi contact $A\,\vec{s}\cdot\vec{I}$ will contribute

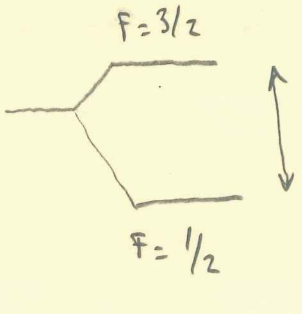
$$\underset{\text{spin-}1/2}{\vec{s}}\cdot\underset{\text{spin-}1\ (D)}{\vec{I}}$$

$\vec{F}\equiv\vec{s}+\vec{I}$; $\vec{s}\cdot\vec{I}=\frac{1}{2}\left[F^2-s^2-I^2\right]$

$\downarrow$

$1/2$ vs $3/2$

$$\underbrace{|\psi_{1s}(0)|^2}_{\text{orbital part}}A\underbrace{\langle\vec{s}\cdot\vec{I}\rangle}_{\text{spin part}}=\frac{A}{2}|\psi_{1s}(0)|^2\underbrace{\left[F(F+1)-I(I+1)-s(s+1)\right]}_{F=1/2\ \to\ -2,\quad F=3/2\ \to\ 1}$$



$|\psi_{1s}(0)|^2 A\,\frac{3}{2}$

3]

$$K_{\alpha\beta} \equiv \int \frac{\overbrace{\varphi_\alpha(\vec r_1)\,\varphi^*_\beta(\vec r_1)}^{\Phi^*(\vec r_1)}\;\overbrace{\varphi^*_\alpha(\vec r_2)\,\varphi_\beta(\vec r_2)}^{\Phi(\vec r_2)}}{|\vec r_1 - \vec r_2|}\, d\vec r_1\, d\vec r_2$$

$$= \int d\vec r_1\, \Phi^*(\vec r_1) \underbrace{\int d\vec r_2 \frac{\Phi(\vec r_2)}{|\vec r_1 - \vec r_2|}}_{\text{Convolution of } \frac{1}{r} \text{ and } \Phi(\vec r)}$$

= product of their Fourier transforms

$$\frac{1}{r} \xrightarrow{F} \frac{4\pi}{k^2}\,, \quad \Phi(\vec r) \xrightarrow{F} \tilde\Phi(\vec k)$$

$$\frac{1}{(2\pi)^3}\int d^3k\, e^{i\vec k\cdot\vec r_1}\,\tilde\Phi(\vec k)\,\frac{4\pi}{k^2}$$

$$\Rightarrow K_{\alpha\beta} = \frac{1}{(2\pi)^3}\int d^3k \underbrace{\int d^3r_1\, e^{i\vec k\cdot\vec r_1}\,\Phi^*(\vec r_1)}_{\tilde\Phi(-\vec k) = \tilde\Phi^*(\vec k)}\,\tilde\Phi(\vec k)\,\frac{4\pi}{k^2}$$

$$= \frac{1}{(2\pi)^3}\int d^3k\, |\tilde\Phi(\vec k)|^2\,\frac{4\pi}{k^2} \geq 0$$

4]

O : $1s^2\ 2s^2\ 2p^4 \xrightarrow[\text{vacancies}]{\text{consider}}$ same as carbon (done in class)

Terms are $^3P_{2,1,0}$, $^1D_2$, $^1S_0$

Since p-shell is more than half-filled (for oxygen)

$\Rightarrow$ highest J is ground term $\Rightarrow$ $^3P_2$ //

F : $1s^2\ 2s^2\ 2p^5 \xrightarrow[\text{vacancy}]{\text{consider}}$ same as B (trivial - single $\bar{e}$)

$L = 1$, $S = 1/2$, $J = 3/2,\ 1/2$

Terms are : $^2P_{3/2}$, $^2P_{1/2}$

More than half-filled (for fluorine)

$\Rightarrow$ highest J is ground term $\Rightarrow$ $^2P_{3/2}$ //