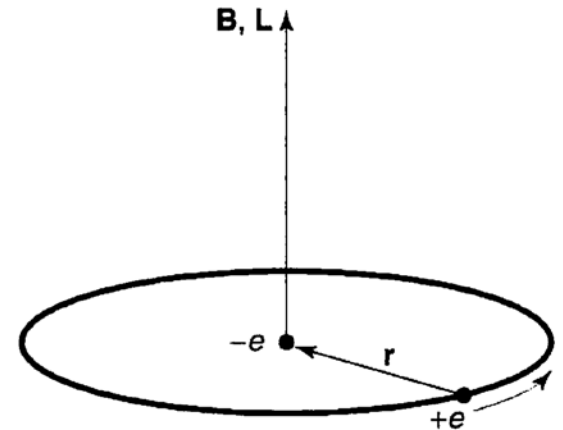


## 7.3.2 Spin-orbit coupling:

From the perspective of the electron, the proton is orbiting around:



From classical electromagnetism a loop of current creates a magnetic field at the center:

$$B = \frac{\mu_0 I}{2r}$$

$$c = 1/\sqrt{\epsilon_0 \mu_0}$$

where the permeability  $\mu_0$  of free space and the permittivity of free space  $\epsilon_0$  are related via:

Side comment: I will send video about this amazing formula.


The current relates with the period  $T$  via:

$$I = e/T$$

and the period  $T$  relates with the angular momentum  $L$  via:

$$L = I \omega = m r^2 \omega$$

$\omega = 2\pi/T$



From study of spins in magnetic fields, Ch. 4, in general:

From previous study of spin:

$$\boldsymbol{\mu}_e = -\frac{e}{m} \mathbf{S}$$

$$H = -\boldsymbol{\mu} \cdot \mathbf{B}$$

From previous page:

$$\mathbf{B} = \frac{1}{4\pi\epsilon_0} \frac{e}{mc^2 r^3} \mathbf{L}$$

Then, overall, classically we obtain the correction called **spin-orbit coupling**:

$$H = \left( \frac{e^2}{4\pi\epsilon_0} \right) \frac{1}{m^2 c^2 r^3} \mathbf{S} \cdot \mathbf{L}$$

Repeating via rigorous math (including the fact that the electron inertia system is accelerating, etc.) leads just to a factor 2 difference:

$$H'_{\text{so}} = \left( \frac{e^2}{8\pi\epsilon_0} \right) \frac{1}{m^2 c^2 r^3} \mathbf{S} \cdot \mathbf{L}$$

**Important statement, without proof:** Because of the  $\mathbf{S} \cdot \mathbf{L}$  term, the Hamiltonian no longer commutes with  $S_z$  (quantum number  $m_s$ ) and  $L_z$  (quantum number  $m_l$ ) but **still commutes with  $L^2$  and  $S^2$  and the total angular momentum  $J^2$  and its projection  $J_z$  (quantum number  $m_j$ ).**

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

$$J^2 = (\mathbf{L} + \mathbf{S}) \cdot (\mathbf{L} + \mathbf{S}) = L^2 + S^2 + 2\mathbf{L} \cdot \mathbf{S}$$

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

**Change of basis required:** from basis with  $(n, l, s, m_l, m_s)$  as quantum numbers to basis with  $(n, l, s, j, m_j)$  as quantum numbers.

$$\frac{\hbar^2}{2} [j(j+1) - l(l+1) - s(s+1)]$$

↖ Fixed to 3/4

Moreover, the expectation value of  $1/r^3$  using H wave functions is:

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

$$\langle H'_{\text{so}} \rangle = \left\langle \left( \frac{e^2}{8\pi\epsilon_0} \right) \frac{1}{m^2 c^2 r^3} \mathbf{S} \cdot \mathbf{L} \right\rangle$$

$\frac{\hbar^2}{2} [j(j+1) - l(l+1) - s(s+1)]$

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

First order in  
perturbation theory

$$E_{\text{so}}^1 = \langle H'_{\text{so}} \rangle = \frac{e^2}{8\pi\epsilon_0} \frac{1}{m^2 c^2} \frac{(\hbar^2/2)[j(j+1) - l(l+1) - 3/4]}{l(l+1/2)(l+1)n^3 a^3}$$

Eqs. from Ch 4 for the  
Bohr radius  $a$  and for  $E_n$ :

$$a \equiv \frac{4\pi\epsilon_0 \hbar^2}{m e^2}$$

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

$$E_n = - \left[ \frac{m}{2\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0} \right)^2 \right] \frac{1}{n^2}$$

In spite of their very different origins, the relativistic and spin-orbit corrections have the same number in front. I.e. **they are of the "same order"**.

Adding both terms naively leads to a long expression

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

Consider  $j=l+1/2$  first. Then  $j(j+1) = (l+1/2)(l+3/2)$ . Careful algebra (HW problem) leads to

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

Consider now  $j=l-1/2$ . Then  $j(j+1) = (l-1/2)(l+1/2)$ . Careful algebra (HW problem) leads to the same

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

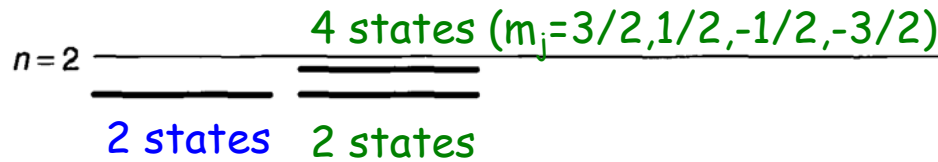
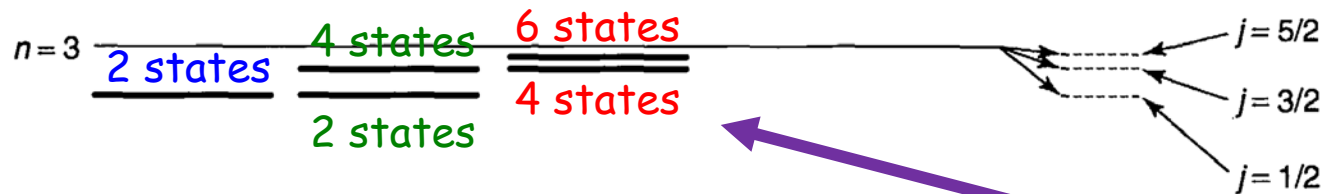
In **HW problem** you will show that order 0 + order 1 gives:

$$E_{nj} = -\frac{13.6\text{eV}}{n^2} \left[ 1 + \frac{\alpha^2}{n^2} \left( \frac{n}{j + 1/2} - \frac{3}{4} \right) \right]$$

where

$$\alpha \equiv \frac{e^2}{4\pi\epsilon_0\hbar c} \approx \frac{1}{137.036}$$

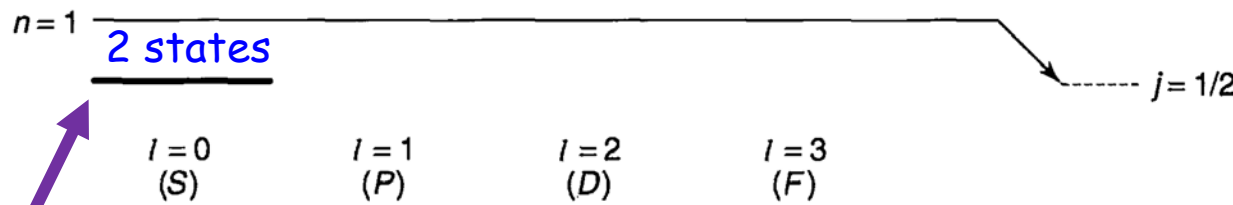
$$E_n = -\left[ \frac{m}{2\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0} \right)^2 \right] \frac{1}{n^2}$$



Originally 10 states because  $l=2$  (5 states) and  $s=1/2$  (2 states)

Originally 6 states because  $l=1$  (3 states) and  $s=1/2$  (2 states)

$j$  runs from  $l+s$  to  $|l-s|$



Originally 2 states because  $l=0$  is 1 state but spin  $s=1/2$  makes it 2 states.

NOTE: this is for the H atom. For He and beyond the e-e repulsion plays a more important role than the fine structure.

## Counting of states repeated for better clarity:

If we consider the "p levels", they have angular momentum  $l=1$ . The spin is  $s=1/2$ . Then, the total angular momentum  $j$  can be  $1+1/2=3/2$  and  $1-1/2=1/2$ .

The original  $l=1$  is 3 states  $m_l = 1, 0, -1$ . The original spin  $s=1/2$  is 2 states  $m_s = 1/2, -1/2$ . Total = 6 states.

The  $j=3/2$  is 4 states  $m_j = 3/2, 1/2, -1/2, -3/2$ . The  $j=1/2$  is 2 states  $m_j = 1/2, -1/2$ . Total = 6 states.

The original 6 degenerate states are simply mixed in special linear combinations to become states with  $j$  sharply defined and different  $j$  projections.

We never create or destroy states by adding perturbations. They just rearrange.