SPIN-ORBIT INTERACTION - FINE STRUCTURE

Let us take an hydrogen atom, but let us look at its motion from the point of view of the electron. If I fix the electron, I see a proton running around it. I can picture the proton as creating a current loop, and use Biot-Savart law to calculate the magnetic field it generates:

$$\vec{B} = \frac{\mu_0 I}{2r} \qquad \text{where } I = \frac{e}{T} \text{ and } T = \text{time for proton to make one turn around electron (or viceversa)}$$

The angular momentum of the electron is:

$$L = mvr = 2\pi m r^2 / T$$

and both L and B point in the same direction. I can finally write:

$$\vec{B} = \frac{1}{4\pi\varepsilon_0} \frac{e}{mc^2 r^3} \vec{L} \qquad \left[c = \frac{1}{\sqrt{\mu_0 \varepsilon_0}} \right]$$

I know that an electron in a magnetic field interacts with it via its spin $\vec{S}$, and the contribution to the Hamiltonian of this interaction is:

$$\Delta E = \mu_B \frac{2}{\hbar} \vec{S} \cdot \vec{B}$$

We proved now that even in the absence of external $\vec{B}$ fields I have a similar phenomenon; its contribution to the Hamiltonian is:

$$\Delta E = \frac{e\hbar}{2m} \cdot \frac{2}{\hbar} \cdot \frac{1}{4\pi\varepsilon_0} \frac{e}{mc^2 r^3} \vec{S} \cdot \vec{L} \cdot \frac{1}{2}$$

$\frac{1}{2}$ ← special factor (Thomas precession) due to fact that coordinate system in which electron at rest is not inertial

Finally:

$$\Delta E = \frac{e^2}{8\pi m^2 c^2 r^3} \vec{S} \cdot \vec{L}$$

SPIN-ORBIT INTERACTION

Remember that $\psi_{n\ell m}(r,\theta,\varphi)$ were the eigenstates of the original Hamiltonian, with well defined quantum numbers n, ℓ, m. Let me now add the spin part, $|\chi\rangle$. Not a big deal, original Hamiltonian was independent of spin, any choice of spinor for my base would work. Let me choose the eigenstates of S_z, $\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\end{pmatrix}$.

Introducing spin doubles the dimension of my eigenstates. Now I have $\psi_{n\ell m}(r,\theta,\varphi)\begin{pmatrix}1\\0\end{pmatrix}$ with quantum numbers n, ℓ, m and $m_s = 1/2$, and $\psi_{n\ell m}(r,\theta,\varphi)\begin{pmatrix}0\\1\end{pmatrix}$ with quantum numbers n, ℓ, m and $m_s = -1/2$.

Now the Hamiltonian contains a term $\propto \vec{S}\cdot\vec{L}$. Question: are ℓ, m and m_s still good quantum numbers? In other words, do L^2, L_z, S_z still commute with the new Hamiltonian contribution?
Some do, some don't... Let us check, keeping in mind that $\vec{L}$ and $\vec{S}$ satisfy similar commutator rules, and they commute between themselves, component by component. We have:

$$[L^2, L_{x,y,z}] = 0 \qquad [L_x, L_y] = i\hbar L_z \quad \text{(cyclic)}$$

$$[S^2, S_{x,y,z}] = 0 \qquad [S_x, S_y] = i\hbar S_z \quad \text{(cyclic)}$$

$$[L_i, S_j] = 0 \quad \text{for any combination of } i \text{ and } j = x, y, z$$

The operator $\vec{L}\cdot\vec{S}$ can be written as $L_x S_x + L_y S_y + L_z S_z$.
Clearly, it commutes with L^2 and S^2, but it does <u>not</u> commute with either L_z or S_z. m and m_s are <u>not</u> good quantum numbers anymore (i.e. I cannot have a state which is a simultaneous eigenstate of the Hamiltonian (with the $\vec{L}\cdot\vec{S}$ piece) and of L_z and S_z)

What about $\vec{J} = \vec{L} + \vec{S}$?

I can write the following expression:

$$J^2 = |\vec{J}|^2 = |\vec{L}+\vec{S}|^2 = L^2 + S^2 + 2\vec{L}\cdot\vec{S}$$

Then, my Hamiltonian becomes proportional to $\frac{|\vec{J}|^2 - |\vec{L}|^2 - |\vec{S}|^2}{2}$. We can also show that: (contribution due to $\vec{L}\cdot\vec{S}$ term)

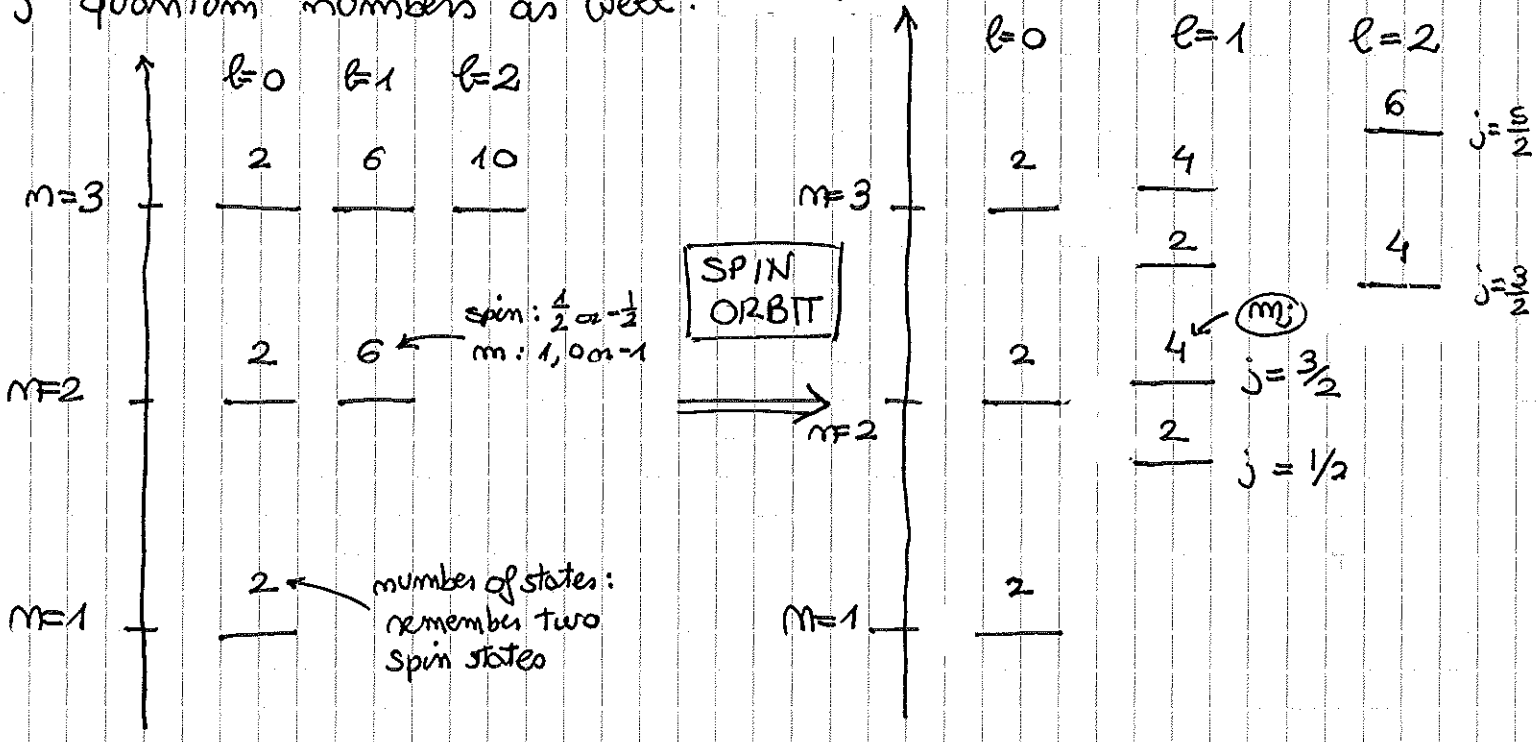
$$[\vec{L}\cdot\vec{S}, J_z] = 0$$

Hence, while my original Hamiltonian had energy eigenstates that were also eigenstates of L^2, L_z, S_z (S^2 is trivially $3\hbar^2/4$, but L^2 is interesting because it identifies the electron orbital angular momentum), now the Hamiltonian with spin-orbit interaction commutes with J^2, L^2, J_z.

$|n\ell m\rangle |s m_s\rangle \Longrightarrow |n\ell j m_j\rangle$ in Dirac's notation (orbital, spin; trivial: spin = 1/2)

$$\Delta E = \frac{e^2}{8\pi\varepsilon_0 m^2c^2}\cdot\frac{1}{r^3}\cdot\vec{L}\cdot\vec{S} = \frac{e^2}{8\pi\varepsilon_0 m^2c^2}\cdot\frac{1}{r^3}\left(|\vec{J}|^2 - |\vec{L}|^2 - |\vec{S}|^2\right)/2 = \frac{e^2\hbar^2/2}{8\pi\varepsilon_0 m^2c^2r^3}\left(j(j+1)-\ell(\ell+1)-\tfrac{3}{4}\right)$$

The energy used to depend on n only: now it depends on the ℓ and j quantum numbers as well: (s is fixed: $\frac{1}{2}$)



How big is this splitting?

$E_1 = -13.6\ eV$

$E_n = -\frac{13.6}{n^2}\ eV$ w/o spin-orbit effect

Let us make a back-of-the-envelope estimation. Our energy correction is: $J^2|n\ell j m_j\rangle = \hbar^2 j(j+1)|n\ell j m_j\rangle$

$$\Delta E_{n\ell j} = \frac{e^2}{8\pi\varepsilon_0 m^2 c^2} \cdot \frac{1}{r^3} \left(j(j+1) - \ell(\ell+1) - s(s+1)\right)\hbar^2/2$$

I write that ΔE depends on n because it contains $1/r^3$, which will give a factor: $\left\langle \frac{1}{r^3} \right\rangle = \langle R_{n\ell}(r)| \frac{1}{r^3} |R_{n\ell}(r)\rangle$ = a function of ℓ and n

Estimation:

$$\Delta E_{n\ell j} \propto \frac{e^2\hbar^2}{16\pi\varepsilon_0 m^2 c^2} \cdot \frac{1}{r^3}$$ (term with j, ℓ, s is just some number of order one)

I can use $\left\langle \frac{1}{r^3} \right\rangle \sim \frac{1}{r_B^3}$ where the Bohr radius $r_B = 5\cdot 10^{-11}\ m$

Also: α = fine structure constant $= \frac{e^2}{4\pi\varepsilon_0\hbar c}$

$$r_B = \frac{4\pi\varepsilon_0\hbar^2}{me^2}$$

$$E_{rest} = mc^2$$

Then: multiply/divide by c^2: $mc^2\left(\frac{e^2}{4\pi\varepsilon_0\hbar c}\right)^4$, with $\frac{e^2}{4\pi\varepsilon_0\hbar c} \sim \alpha^4$

$$\Delta E_{n\ell j} \propto \frac{e^2\hbar^2}{16\pi\varepsilon_0 m^2 c^2} \cdot \frac{m^3 e^6}{(4\pi\varepsilon_0\hbar^2)^3} \propto \frac{me^8}{(4\pi\varepsilon_0\hbar)^4 c^2} = \alpha^4 E_{rest}$$

$\alpha = \frac{1}{137}$, $E_{rest} = 0.5\ MeV$ ($\uparrow$ mega: 10^6) $\Rightarrow \Delta E_{n\ell j} \approx 10^{-3}\ eV$