Spin Orbit Interactions PhL 11.16.07

These notes are based on Livesey more or less. I later realized that Schiff has all this stuff perhaps in a clearer form, and of course Condon Shortley and Harnwell have it too, as to various other books I own.

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1. Electron spin-orbit interaction. On page 230 of Livesey, we see a discussion which goes as follows: you can think of the electron at rest with the nucleus flying around it. If the nucleus has velocity v, then it creates a magnetic field at the site of the electron.

Purcell page 214 equation 56 + 60 says the size of this field (in cgs units) is $\mathbf{B} = \gamma\,(\mathbf{v}/c) \times \mathbf{E}$ where $\mathbf{E}$ is $-q\mathbf{r}/r^3$, the static field of the nucleus in it rest frame (this is a non-relativistic approximation. We can set this $\gamma = 1$ if v is non-relativistic (but let's not do that). Thus, we have $\mathbf{B} = -(\gamma Ze/c)\,\mathbf{v} \times \mathbf{r}/r^3$ being seen by the electron.

You get this same result from the Biot-Savart law on page 201 of Purcell if you imagine the current as a cylinder dA area density ρ length dx making a current that is $I = \rho dA dx/dt = \rho\, dA\, v$. Then set $dq = \rho dA dx$ and $d\boldsymbol{\ell} = \hat{\mathbf{v}}\, dx$ and the result falls out (without the γ since non-rel) .

Now we know that $\mathbf{L} = \mathbf{r} \times \mathbf{p} = \mathbf{r} \times (\gamma m_e \mathbf{v})$ for our electron, so we can then replace $\mathbf{v} \times \mathbf{r} = -\mathbf{L}/\gamma m_e$ to get $\mathbf{B} = -(\gamma Ze/c)\,\mathbf{v} \times \mathbf{r}/r^3 = +(Ze/m_e c)\,\mathbf{L}/r^3$. This L is in fact the angular momentum of the electron around the proton, and we are just using it to replace our $\mathbf{v} \times \mathbf{r}$ factor.

Now, back to our electron. Suppose it has magnetic moment $\boldsymbol{\mu}_e = \gamma_e \mathbf{S}$ (Levitt gyro γ). We can then say that the interaction Hamiltonian is

$$H' = -\boldsymbol{\mu}_e \bullet \mathbf{B} = -\gamma_e \mathbf{S} \bullet (Ze/m_e c)\,\mathbf{L}/r^3 = -\gamma_e (Ze/m_e c)\,\mathbf{L} \bullet \mathbf{S}/r^3$$

and we thus have a *classical derivation* for the **spin-orbit interaction** seen by the electron. If we now look at Livesey page 230, he says that $\gamma_e = -e/m_e$ so the result would then be

$$H' = -\boldsymbol{\mu}_e \bullet \mathbf{B} = +(Ze^2/m_e^2 c)\,\mathbf{L} \bullet \mathbf{S}/r^3$$

What do things look like in mks units? I am not sure what the field transform equations look like in mks units, so I don't know how to replace "$\mathbf{B} = \gamma\,(\mathbf{v}/c) \times \mathbf{E}$ " above. But I do know what the Biot-Savart looks like in mks units. It has an extra $\mu_0/4\pi$ and is missing the 1/c. So to get our induced B field in mks units, we need to make the replacement $1/c \rightarrow (\mu_0/4\pi)$. We then get

$$\mathbf{B}_{mks} = (\mu_0/4\pi)(Ze/m_e)\,\mathbf{L}/r^3 = (1/4\pi\varepsilon_0)(Ze/m_e c^2)\,\mathbf{L}/r^3 \qquad // \ \mu_0 = 1/(\varepsilon_0 c^2)$$

and then our interaction Hamiltonian would be

$$H' = -\boldsymbol{\mu}_e \bullet \mathbf{B} = -\gamma_e (1/4\pi\varepsilon_0)(Ze/m_e c^2)\, \mathbf{L}\bullet\mathbf{S} / r^3 = (1/4\pi\varepsilon_0)(Ze^2/m_e^2 c^2)\, \mathbf{L}\bullet\mathbf{S} / r^3 \qquad // \ \gamma_e = -e/m_e$$

and this last result agrees with Livesey last equation on page 230. Note that L and S include $\hbar$ factors as presented here, so Livesey has $L = G_\ell$ and the same for spin. You could write $\mathbf{L} = \hbar\boldsymbol{\ell}$ and $\mathbf{S} = \hbar\mathbf{s}$ but let's not do that right now.

Now in the above derivation (using the first method in cgs units), in computing **B** we used $\mathbf{E} = -Zq\mathbf{r}/r^3$. If you have some *other* central potential $\phi(r)$, then $\mathbf{E} = -\nabla\phi = -\mathbf{r}/r\, \partial_r\phi$. So to handle this situation, we want to make the replacement $-q\mathbf{r}/r^3 \rightarrow -\mathbf{r}/r\, \partial_r\phi$ which says $q/r^3 \rightarrow (1/r)\partial_r\phi$. If we make this replacement in our results above, we get,

$$H' = -\boldsymbol{\mu}_e \bullet \mathbf{B} = -\gamma_e (1/m_e c)\, \mathbf{L}\bullet\mathbf{S}\, [\, (1/r)\partial_r\phi\,] = +(e/m_e^2 c)\, \mathbf{L}\bullet\mathbf{S}\, [\, (1/r)\partial_r\phi\,] \quad // \text{ cgs}$$

Correction: In the above discussion, we have given a very crude derivation of the interaction Hamiltonian for the spin-orbit interaction. We argued that the electron sees a moving proton which makes a B field which then interacts with the electron's spin. To solve this problem correctly, you need to do it relativistically with the 4-spinors and all that stuff. This seems to be done in my Harnwell-Stephens book around page 177 and a few pages preceding. The results they get seem to differ by a factor of 2 from those I got above by my simple derivation. Livesey does comment that his result is not "reliable", but he has other things in mind when he says that.

At first I thought this factor of 2 had to do with the definition of **S**, but I see that everybody really does S the same way, so values S_z has eigenvalues $\pm\, \hbar/2$. So here is the result from the relativistic calculation which I quote from HS page 177: (these appear right next to each other in HS, mks units)

$$H' = (1/\mathbf{8}\pi\varepsilon_0)(Ze^2/m_e^2 c^2)\, \mathbf{L}\bullet\mathbf{S} / r^3 \qquad // \text{ HS page 177}$$

$$H' = (\mathbf{1/2})(1/m_e^2 c^2)\, \mathbf{L}\bullet\mathbf{S}\, [\, (1/r)\partial_r V\,] \qquad // \text{ HS page 177, V is potential energy} = e\phi$$

For corroboration, the second equation above appears in Condon Shortley (CS) page 120, where U is really $e\phi$, not ϕ.

Comment added 9.16.08: I think this factor of 2 is a relativistic effect related to Thomas Precession, but I don't know the details. It is caused by the fact that when one derives the L•S coupling classically as done above, one pretends the electron is at rest and the proton moves around it making its B field. But in fact the electron is constantly accelerating and is therefore not an "inertial frame" and so does not have a simple connection to that rest frame. When you account for this constant acceleration with relativity in mind, you obtain the factor of 2. This factor is not a function (it seems) of how fast the electron is going. It arises from the fact that boosts don't commute.

Comment: If you do the full relativistic solution of the hydrogen atom, the fact that the electrons have something called "spin" just "falls out" from the theory, it does not have to be a separate *ad hoc* postulate. Secondly, in terms of this spin, if you take the non-relativistic limit of the Hamiltonian, you find that the Hamiltonian has an **L•S** term which we call "the spin-orbit interaction". So spin and the L•S coupling are both "relativistic effects".

2. Nuclear spin-orbit interaction. Now by the exact same argument, the nucleus sees the electron flying around and sees $\mathbf{B} = (-e/m_e c)\, \mathbf{L}\, /r^3$ where e >0 in our notation, and of course -e replaces Ze as the charge. Then if the nucleus has spin I, we can write $\boldsymbol{\mu}_N = \gamma_N \mathbf{I}$ [see Levitt p 175] to get

$$H'' = -\boldsymbol{\mu}_N \bullet \mathbf{B} \;\; = -\gamma_N \mathbf{I} \bullet (-e/m_e c)\, \mathbf{L}\, /r^3 \;\; = +\gamma_N (e/m_e c)\, \mathbf{I} \bullet \mathbf{L} \,/\, r^3$$

3. Spectroscopic Notation and Fine Structures . When you solve the hydrogen atom problem in non-rel QM, you get the energy formula shown in 7.7.6 in Livesey page 211 where the main quantum number is $n = \ell + \rho + 1$. We know the ℓ can have values 0,1,2,3 since it is angular momentum arising from variable separation. The ρ number can range 0,1,2... and is a power which allows a series to terminate in the r variable part of the solution. Thus, n has the range 1,2... So the question is how to you *organize* the quantum numbers? The usual way is as follows: pick n=1, then must have $\ell = 0$. Next, pick n=2. Here you can have $\ell = 0$ and 1, and so on. Thus, once you pick n, **ℓ can range ℓ = 0,1,2....(n-1)**.

This leads at once to the **table on page 220 of Livesey**, just look at the n and ℓ columns. The number n is associated with an "x-ray letter" like k,ℓ,m,n,o which are historical letters from before the atom was solved. The angular momentum "subshells" have the famous names s,p,d,f,g for ℓ = 0,1,2,3,4. The number of electrons each shell can hold is shown at the right. This table seems pretty reasonable. This table is showing the various energy levels of the hydrogen atom ONLY. Those states with the same value of n are all degenerate, according to our hydrogen E_n result.

When you start increasing Z and adding electrons for "form the periodic table", you start having the **shielding** issue. Electrons in higher ℓ orbitals see a shielded nuclear charge so they see a smaller effective value for Z. In our energy formula page 211, smaller Z means a smaller negative energy, which means the energy level moves *up* for a large-ℓ state. Page 221 is showing what happens. On the right, imagine that all the orbitals are n-degenerate (although not drawn that way). This is what the energy levels would be for atoms if there were no shielding effect. When shielding is accounted for, the higher ℓ levels are pushed up and we get the scale shown at the far left. The n-degeneracy is broken, and the n levels are in fact interleaved. The levels shown at the left of 221 show the energy levels for the "valence electron" of light atoms. For example, consider an atom with Z = 6. You fill the 1s and the 2s and you have two "valence electrons" in the 2p (where there is room for up to 6). Presumably, the height of the various energy levels on the left really is the set of energy levels for a Z = 6 atom with 6 electrons installed in the bottom levels. The unoccupied levels would control the "spectrum" of this atom if photons are fired at it. Of course this is not really true, because as you build up, with each next atom all the levels are going to shift a little bit. I think this is what the figure is showing. As you build up, you move to the right and the levels are shifting. So a vertical line in this picture at some Z would show you the true spectral levels for that particular atom, and you understand that the lowest Z states are filled.

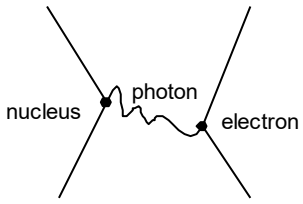
Now comes the **next complication which is spin**. Look at page 229. For each (n,ℓ) orbital level, we have some value of ℓ, and the electron has its s = 1/2. Since only J is a "true quantum number" (Casimir under O3 rotations), you really need to specify your levels by n and J. Of course $j = \ell + 1/2$ and ℓ - 1/2. We are talking about the quantum states of hydrogen with spin accounted for. The spectroscopic notation used for the true energy levels of such an atom is of the form $n^2\, \ell_j$ but instead of actually putting the ℓ value, we put its letter S,P,D and so on.

At the bottom of page 231 Livesey states the **relativistic solution to the hydrogen atom**, and you see two quantum numbers υ and j . On page 232 he does a series for this thing and reaches this interesting conclusion: the energy formula (to first order) is the same the Bohr no-spin solution, except instead of n

$= \ell + \rho + 1$, you have $n = j + \upsilon + 1/2$ where $\upsilon = 0,1,2..$. So you organize your levels now by first picking an n value, then list of the j's you can have for that n. If n=1, then j=1/2. If n=2, j = 1/2, 3/2. and so on. In other words, j = 1/2, 3/2, ... (2n-1)/2. Livesey then looks at the "second order" term as shown in 7.10.7 page 232 where we now have a bracket factor multiplying our Bohr-like result. For small values of j and n (at least), this factor is slightly larger than 1, so energy levels are pushed *down*. And for a given n value, the different j values are split apart with larger j causing a smaller [..] factor pushing the level up. This then completely explains the first two columns of the drawing on page 233. The middle column shows the true states of hydrogen when spin is incorporated in the Dirac theory. Notice that spectroscopic states with the same j are degenerate as the formula says should be the case.

The Dirac splitting of the Bohr levels is called **"fine structure"** and the size of the splittings is on the order of 45 μeV, so is very small compared to the 1 eV scale of the levels overall. Claim is that this corresponds to 11 GHz, compared to the optical frequencies of the main levels.

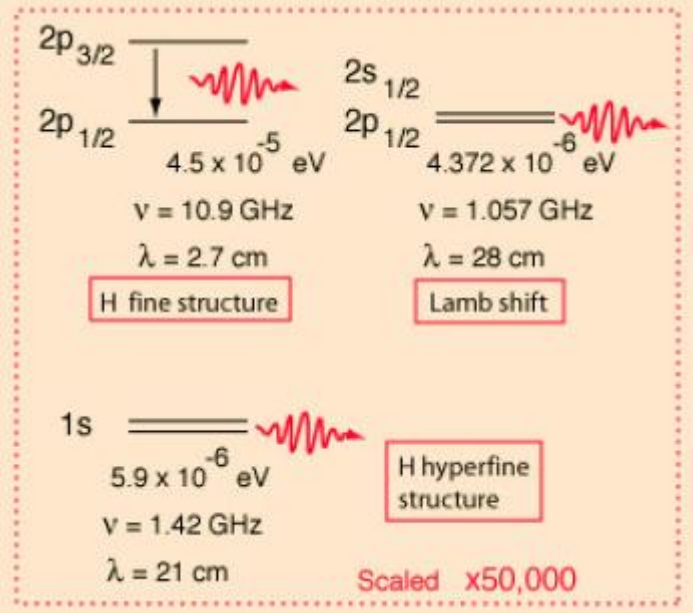
So, we started with Bohr theory, and then we added spin with the Dirac theory. The **next** level of sophistication is that we have to think of the hydrogen atom interaction as being represented by this Feynman diagram:



If you continue doing perturbation theory and do all the 4-vertex Feynman diagrams (see below), you pick up extra corrections to the spectrum of hydrogen. For example, there are two vertex correction diagrams and one diagram with a virtual pair on the photon. You might think these corrections must be down by factor α^2 or even α^4, but in fact they are weaker than the fine structure splitting by only a factor of 1/10. [We also get corrections to the electron's magnetic moment]

In any event, we end up with a splitting of the two j=1/2 levels (S and P) at the n=2 level in the picture on page 233, and this is the **Lamb Shift**, frequency 1.057864 GHz.

In addition to the Lamb shift, the effect of the **nuclear spin** causes **another splitting** which is shown in the lower right in the page 233 picture. This arises from the **I•L** terms (see section 2 above) and its size is similar to the Lamb shift size, about 1.42 GHz. Here is a little graphic:



I think only this nuclear effect is called the **"hyperfine structure"**, but the Lamb shift is a similar size as you see here. [Comment added: probably you can estimate the nuclear splitting of the hyperfine structure using the Levitt style through-space dipole-dipole coupling and avoid Feynman diagrams.]

4. Facts about Edward Purcell // (August 30, 1912 – March 7, 1997)

FROM http://www.news.harvard.edu/gazette/1998/04.09/FacultyofArtsan.html

(1) During the war Purcell headed the group working on very short wavelength radar at the MIT Radiation Laboratory, where microwave radar was being urgently developed to contribute decisively to the Allied victory.

(2) In **1945** Purcell (with Pound and Torrey) observed nuclear magnetic resonance (NMR), in an after-hours experiment while still completing work on the classic *27-volume* series of books on radar. Though initially used in physics, NMR has been applied powerfully as an analytic method for elucidating chemical structure and materials properties. The Nobel prize winning discovery is also the basis of medical resonance imaging (or MRI), now routinely used as an elegant and non-invasive diagnostic tool, producing beautifully detailed images of the body's interior.

[Nuclear magnetic resonance was first described and measured in molecular beams by Isidor **Rabi** in 1938.[1] Eight years later, in 1946, Felix **Bloch** and Edward Mills **Purcell** refined the technique for use on liquids and solids, for which they shared the Nobel Prize in physics in 1952.]

(3) In 1951 Purcell (with his student Harold Ewen) was the **first to detect the 21 cm hydrogen hyperfine emission** from galactic neutral atomic hydrogen, radioastronomy's first spectral line. This had been predicted seven years earlier by van de Hulst and Oort at Leiden, whose group had to settle for second place. In a most gentlemanly gesture, Purcell and Ewen insisted that Nature delay publication of

their own paper until the Dutch group had a chance to confirm their results and have them published simultaneously. Hydrogen line observations soon produced the first maps of our galaxy's spiral arms, until then hidden from human view by dust; they have been a major tool of radioastronomy ever since.

(4) Purcell's **other** contributions to these fields included:

a comprehensive theory of nuclear magnetic **relaxation** (with Bloembergen and Pound - the famous "BPP" paper, one of the most cited references in physics);

the concept of **negative spin temperatures** (with Pound), which was a precursor to the maser and laser;

improved **spin-echo** techniques (with Carr);

and explanations of the absorption and scattering of starlight by **interstellar grains**.

With Ramsey he was the first to question the conventional assumption (later disproved) that all particle forces are **parity** symmetric.

With Berg he applied physics to **biological** problems, in their description of the physics of chemoreception and in his **classic paper** (in The American Journal of Physics) "Life at Low Reynolds Number," a life whose locomotion is dominated by viscosity.

In that same journal his monthly "Back of the Envelope" problems challenged and delighted a large audience of physicists.

5. More on the Lamb shift http://www.pha.jhu.edu/~rt19/hydro/node8.html

According to Dirac and Schrödinger theory, states with the same *n* and *j* quantum numbers but different *l* quantum numbers ought to be degenerate. However, a famous experiment by Lamb and Retherford in 1947 showed that the $2s_{1/2}(n=2, l=0, j=1/2)$ and $2p_{1/2}(n=2, l=1, j=1/2)$ states of the hydrogen atom were not degenerate, but that the *s* state had slightly higher energy by an amount now known to be $E/h = 1057.864\text{MHz}$. The effect is explained by the theory of quantum electrodynamics, in which the electromagnetic interaction itself is quantized. Some of the effects of this theory which cause the Lamb shift are shown in the Feynman diagrams of figure 5.

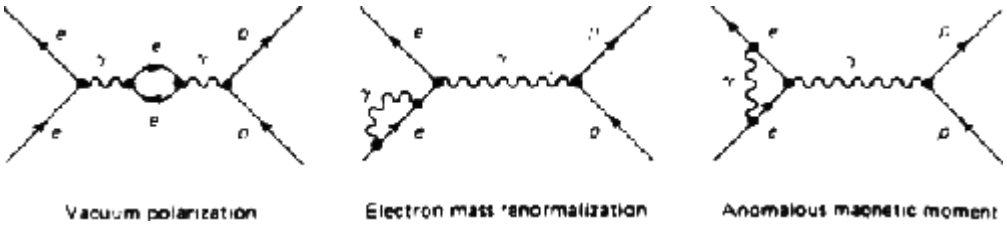


Figure 5: Feynman loop diagrams showing some effects that contribute to the Lamb shift.

Table 3 shows how much each of these contribute to the splitting of $2s_{1/2}$ and $2p_{1/2}$.

Effect	Energy contribution
Vacuum polarization	-27 MHz
Electron mass renormalization	+1017 MHz
Anomalous magnetic moment	+68 MHz
Total	+1058 MHz

Table 3: Contribution of different effects to the energy splitting of $2s_{1/2}$ and $2p_{1/2}$ in hydrogen. Numbers are given in units of frequency $\nu = E/h$.

The most important effect is illustrated by the center diagram, which is a result of the fact that the ground state of the electromagnetic field is not zero, but rather the field undergoes ``vacuum fluctuations" that interact with the electron. Any discussion of the calculation is beyond the scope of this paper, so the answers will merely be given. For *l*=0,

$$\Delta E_{Lamb} = \alpha^5 mc^2 \frac{1}{4n^3}\{k(n,0)\}, \qquad (73)$$

where *k*(*n*,0) is a numerical factor which varies slightly with *n* from 12.7 to 13.2. For $l \neq 0$,

$$\Delta E_{Lamb} = \alpha^5 mc^2 \frac{1}{4n^3}\left\{k(n,l) \pm \frac{1}{\pi(j+\frac{1}{2})(l+\frac{1}{2})}\right\} \qquad (74)$$

for $j = l \pm 1/2$, where *k*(*n*,*l*) is a small numerical factor <0.05 which varies slightly with *n* and *l*. Notice that the Lamb shift is very small except for *l*=0.

Randy Telfer

6. "Single electron" atoms

Atoms that have one valence electron like Na (alkali metals) behave pretty much according to our hydrogen Bohr model, as if the nucleus + all the closed shells act as an effective shielded nucleus. Of course you want to include the spin complication. If you look near the left edge of the figure page 221 Livesey, you see the ordering of energy levels (Z = 11, so $(1s)^2(2s)^2(2p)^6(3s)^1$, see page 494) that would apply for Na's valence electron. If you make a picture where you put the different ℓ states in different columns, you get that shown on page 235. This picture does not show the lower filled levels. For each ℓ value (column) the two spin states are shown giving the two j values. The purpose of using columns is that the normal electric-dipole photon transition does not see spin and requires $\Delta\ell = 1$ (see p 249), so you cannot have a dipole transition within a column. Each arrow in this picture corresponds to a "line" in the Na spectrum. That is, heat up Na, and the valence electron bounces around in the states shown. I think atoms with one "hole" in shell behave in a similar manner.

7. "Two electron" atoms : LS and jj coupling schemes.

Think Helium, positronium, or something like Mg (Z=12) where there are in effect *two* valence electrons. How do you solve *this* problem in QM? And what does this have to do with the **L•S** Hamiltonian term?

The idea is to do some kind of perturbation theory because exact solutions are too hard. If you ignore the spin-orbit interaction, then all six quantum numbers J,L,S and their M_z values are all conserved, where these are somehow "total quantities". The question is : how to you make these totals?

There are two general schemes known as LS and jj coupling.

In the LS (Russell-Sanders, used for light elements where LS is weak relative to coulomb) scheme for two electrons in an atom, you would do $\mathbf{L} = \boldsymbol{\ell}_1 \otimes \boldsymbol{\ell}_2$ to find the allowed L values for the 2-electron combined system. Similarly, do $\mathbf{S} = \mathbf{s}_1 \otimes \mathbf{s}_2$ to find the legal S values (which are going to be S = 0 and S = 1 for a 2-electron atom). Then for each LS combination, compute $\mathbf{J} = \mathbf{L} \otimes \mathbf{S}$. You can label your states this way: $|JLSM_J\rangle$ if you want. This then allows the same "spectroscopic notation" that is used in the single-electron atoms.

Example: for Helium, you have S = 0 and S = 1 so you can separate your spectrum into two parts as shown page 240. These even have names: parhelium and orthohelium. Page 239 shows how you would list off all the S=0 states. You put your second electron in various orbitals and for each case you see what L values are allowed. In all these states, one electron is in the $\boldsymbol{\ell}_1 = 0$ ground state, so we basically then just have $\mathbf{L} = \boldsymbol{\ell}_2$. We also have $\mathbf{J} = \mathbf{L}$ since S = 0. So you see the states in the picture on the left side of p 240.

You then do the same idea for the S=1 situation. Everything is as before, but now $\mathbf{J} = \mathbf{L} \otimes \mathbf{1}$ so we have in general three J values for each L (except for L=0). Due to the selection rule $\Delta S = 0$ for dipole, the two spectra tend to remain separate from each other.

In the jj coupling scheme (used for heavy elements where L*S is relatively strong), we do things differently. We do $\mathbf{j}_1 = \boldsymbol{\ell}_1 \otimes \mathbf{s}_1$ for one electron, and then for the other electron it is $\mathbf{j}_2 = \boldsymbol{\ell}_2 \otimes \mathbf{s}_2$. Then we do $\mathbf{J} = \mathbf{j}_1 \otimes \mathbf{j}_2$. In this scheme we can label the states $|\, J\, j_1\, j_2\, M_J \rangle$.

The claim is that in light elements, the spin-orbit is weak, so the notion of a conserved L and S is viable, so these are pretty good quantum numbers. In heavy elements, spin-orbit is as strong as the electrostatic interaction so it does not even make sense to talk about L , for example. I see that the L*S magnitude increases with Z, whereas the electronic stuff is shielded? Well, I don't really see the reason for the different regimes of LS and jj, but at least I have a vague idea what they are talking about.