# ZEEMAN EFFECT: STRONG FIELD

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 6.22.

In the weak field Zeeman effect, the splitting of the energy levels due to the external field $\mathbf{B}_{ext}$ is treated as a subsidiary perturbation on top of the stronger perturbation due to spin-orbit coupling. This means that we use the 'good' quantum numbers appropriate to spin-orbit coupling to determine the eigenstates used in calculating the Zeeman perturbation.

If the situation is inverted, so that $\mathbf{B}_{ext}$ is strong enough to disrupt spin-orbit coupling, then the 'good' quantum numbers become those with which the Zeeman hamiltonian term commutes, and we need to evaluate the spin-orbit hamiltonian using these eigenstates. The Zeeman hamiltonian term is

$$H'_Z = -(\mu_L + \mu_S) \cdot \mathbf{B}_{ext} \tag{0.1}$$

If we direct $\mathbf{B}_{ext}$ along the $z$ axis, then

$$H'_Z = \frac{e}{2m}(L_z + 2S_z) B_{ext} \tag{0.2}$$

In this case, $\mathbf{J}$ and $j_z$ do not commute with $H'_Z$ so we can take as the eigenstates $|n\ell\ell_z s_z\rangle$. (I'm using the notation $\ell_z$ and $s_z$ to refer to the $z$ quantum numbers rather than the more traditional $m_\ell$ and $m_s$ in order to avoid confusion with the mass $m$ and because it seems a more transparent notation.) The Zeeman correction to the energy is therefore

$$E_{Z1} = \langle n\ell\ell_z s_z | H'_Z | n\ell\ell_z s_z \rangle \tag{0.3}$$

$$= \frac{e\hbar}{2m}(\ell_z + 2s_z) B_{ext} \tag{0.4}$$

$$= \mu_B (\ell_z + 2s_z) B_{ext} \tag{0.5}$$

The problem is that in order to add in the fine structure correction (which is now the minor perturbation on top of the Zeeman effect), we need to work out the energy correction relative to these eigenstates. Again, this is a bit of a fudge, since although the relativistic hamiltonian correction does

commute with $L_z$ and $S_z$, the spin-orbit hamiltonian doesn't. Just as in the weak field case, we'll do the calculation anyway and see what we get.

What we want then is the fine structure energy correction $E_{fs1}$:

$$E_{fs1} = \langle n\ell\ell_z s_z | H'_{rel} + H'_{so} | n\ell\ell_z s_z \rangle \tag{0.6}$$

Because the relativistic term commutes with $L_z$ and $S_z$, we can just quote the result from before:

$$\langle n\ell\ell_z s_z | H'_{rel} | n\ell\ell_z s_z \rangle = -\frac{E_{n0}^2}{2mc^2}\left(\frac{4n}{\ell+\frac{1}{2}} - 3\right) \tag{0.7}$$

The spin orbit term is what causes the problems. We need to calculate

$$E_{so1} = \langle n\ell\ell_z s_z | H'_{so} | n\ell\ell_z s_z \rangle \tag{0.8}$$

$$= \frac{e^2}{8\pi\varepsilon_0 m^2 c^2}\left\langle \frac{1}{r^3} \right\rangle \langle \mathbf{S}\cdot\mathbf{L} \rangle \tag{0.9}$$

The average $\left\langle \frac{1}{r^3} \right\rangle$ is the same as before, since it depends only on $n$ and $\ell$:

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{\ell\left(\ell+\frac{1}{2}\right)(\ell+1)n^3a^3} \tag{0.10}$$

When we worked out $\langle \mathbf{S}\cdot\mathbf{L} \rangle$ earlier, we were using eigenstates of $J^2$ and $J_z$ which we can't use here. We can however say:

$$\langle \mathbf{S}\cdot\mathbf{L} \rangle = \langle S_x L_x + S_y L_y + S_z L_z \rangle \tag{0.11}$$

Because we're taking $\mathbf{B}_{ext}$ along the $z$ axis and $\mathbf{S}$ and $\mathbf{L}$ precess about the $z$ axis, the average of their $x$ and $y$ components will be zero, so we can take

$$\langle \mathbf{S}\cdot\mathbf{L} \rangle = \langle S_z L_z \rangle = \hbar^2 s_z \ell_z \tag{0.12}$$

Therefore we get

$$E_{so1} = \frac{e^2\hbar^2 s_z\ell_z}{8\pi\varepsilon_0 m^2 c^2}\frac{1}{\ell\left(\ell+\frac{1}{2}\right)(\ell+1)n^3a^3} \tag{0.13}$$

Putting it all together, we have

$$E_{fs1} = -\frac{E_{n0}^2}{2mc^2}\left(\frac{4n}{\ell+\frac{1}{2}} - 3\right) + \frac{e^2 s_z\ell_z}{8\pi\varepsilon_0 m^2 c^2}\frac{1}{\ell\left(\ell+\frac{1}{2}\right)(\ell+1)n^3a^3} \tag{0.14}$$

To simplify this, we can express things in terms of the fine structure constant $\alpha$:

$$\alpha \equiv \frac{e^2}{4\pi\varepsilon_0\hbar c} \tag{0.15}$$

$$a = \frac{4\pi\varepsilon_0\hbar^2}{me^2} = \frac{\hbar}{\alpha mc} \tag{0.16}$$

$$E_{n0} = -\frac{\alpha^2 mc^2}{2n^2} \tag{0.17}$$

We then get

$$E_{fs1} = -\frac{E_{10}^2}{2n^4 mc^2}\left(\frac{4n}{\ell+\frac{1}{2}} - 3\right) + \frac{\alpha^4 mc^2}{2n^3}\frac{\ell_z s_z}{\ell\left(\ell+\frac{1}{2}\right)(\ell+1)} \tag{0.18}$$

$$= \frac{E_{10}\alpha^2}{4n^4}\left(\frac{4n}{\ell+\frac{1}{2}} - 3\right) - \frac{E_{10}\alpha^2}{n^3}\frac{\ell_z s_z}{\ell\left(\ell+\frac{1}{2}\right)(\ell+1)} \tag{0.19}$$

$$= \frac{E_{10}\alpha^2}{n^3}\left(\frac{1}{\ell+\frac{1}{2}} - \frac{3}{4n} - \frac{\ell_z s_z}{\ell\left(\ell+\frac{1}{2}\right)(\ell+1)}\right) \tag{0.20}$$

$$= \frac{13.6\text{ eV}}{n^3}\alpha^2\left[\frac{3}{4n} - \frac{\ell(\ell+1)-\ell_z s_z}{\ell\left(\ell+\frac{1}{2}\right)(\ell+1)}\right] \tag{0.21}$$

The complete energy formula for the strong field Zeeman effect is then

(0.22)

$$E_n = E_{n0} + E_{fs1} + E_{Z1}$$

(0.23)

$$= -\frac{13.6\text{ eV}}{n^2}\left[1 - \frac{\alpha^2}{n}\left(\frac{3}{4n} - \frac{\ell(\ell+1)-\ell_z s_z}{\ell\left(\ell+\frac{1}{2}\right)(\ell+1)}\right)\right] + \mu_B\left(\ell_z + 2s_z\right)B_{ext}$$

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