

ZEEMAN EFFECT FOR N = 3: GENERAL CASE

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 6.26 (general field).

To complete our analysis of the $n = 3$ line in the Zeeman effect, we need to calculate the general degenerate perturbation matrix W . We'll follow the same procedure as that for $n = 2$ (except this time I'll do it for only one set of eigenstates!) and use the $|n\ell jj_z\rangle$ states as the basis for the matrix elements. We now have a total of 18 degenerate unperturbed states (the 8 we had for $n = 2$ with $\ell = 0, 1$ plus 10 for $\ell = 2$).

The eigenvalue equations we need to work out W are

$$H'_{fs} |n\ell jj_z\rangle = \frac{13.6 \text{ eV}}{n^3} \alpha^2 \left(\frac{3}{4n} - \frac{1}{j + \frac{1}{2}} \right) |n\ell jj_z\rangle \quad (1)$$

$$H'_Z |\ell\ell_z\rangle |ss_z\rangle = \mu_B B_{ext} (\ell_z + 2s_z) |\ell\ell_z\rangle |ss_z\rangle \quad (2)$$

Here $n = 3$, so we'll rewrite these equations to make them a bit more compact:

$$H'_{fs} |2\ell jj_z\rangle = \frac{13.6 \text{ eV}}{27} \alpha^2 \left(\frac{1}{4} - \frac{4}{4(j + \frac{1}{2})} \right) |n\ell jj_z\rangle \quad (3)$$

$$= \frac{13.6 \text{ eV}}{108} \alpha^2 \left(1 - \frac{4}{j + \frac{1}{2}} \right) |n\ell jj_z\rangle \quad (4)$$

$$\equiv \gamma \left(1 - \frac{4}{j + \frac{1}{2}} \right) |n\ell jj_z\rangle \quad (5)$$

$$H'_Z |\ell\ell_z\rangle |ss_z\rangle = \mu_B B_{ext} (\ell_z + 2s_z) |\ell\ell_z\rangle |ss_z\rangle \quad (6)$$

$$\equiv \beta (\ell_z + 2s_z) |\ell\ell_z\rangle |ss_z\rangle \quad (7)$$

Note that the γ here is different from the one we used in the $n = 2$ case.

Since the $\ell = 0$ and $\ell = 1$ states are the same as in the $n = 2$ case, their decomposition into $|\ell\ell_z\rangle |ss_z\rangle$ states via Clebsch-Gordan coefficients is the same, so the matrix elements of H'_Z are the same as well. As a reminder, the $\ell = 0$ and $\ell = 1$ states are:

$$\psi_1 = \left| 30 \frac{1}{2} \frac{1}{2} \right\rangle = |00\rangle \left| \frac{1}{2} \frac{1}{2} \right\rangle \quad (8)$$

$$\psi_2 = \left| 30 \frac{1}{2} - \frac{1}{2} \right\rangle = |00\rangle \left| \frac{1}{2} - \frac{1}{2} \right\rangle \quad (9)$$

$$\psi_3 = \left| 31 \frac{3}{2} \frac{3}{2} \right\rangle = |11\rangle \left| \frac{1}{2} \frac{1}{2} \right\rangle \quad (10)$$

$$\psi_4 = \left| 31 \frac{3}{2} - \frac{3}{2} \right\rangle = |1-1\rangle \left| \frac{1}{2} - \frac{1}{2} \right\rangle \quad (11)$$

$$\psi_5 = \left| 31 \frac{3}{2} \frac{1}{2} \right\rangle = \sqrt{\frac{2}{3}} |10\rangle \left| \frac{1}{2} \frac{1}{2} \right\rangle + \sqrt{\frac{1}{3}} |11\rangle \left| \frac{1}{2} - \frac{1}{2} \right\rangle \quad (12)$$

$$\psi_6 = \left| 31 \frac{1}{2} \frac{1}{2} \right\rangle = -\sqrt{\frac{1}{3}} |10\rangle \left| \frac{1}{2} \frac{1}{2} \right\rangle + \sqrt{\frac{2}{3}} |11\rangle \left| \frac{1}{2} - \frac{1}{2} \right\rangle \quad (13)$$

$$\psi_7 = \left| 31 \frac{3}{2} - \frac{1}{2} \right\rangle = \sqrt{\frac{1}{3}} |1-1\rangle \left| \frac{1}{2} \frac{1}{2} \right\rangle + \sqrt{\frac{2}{3}} |10\rangle \left| \frac{1}{2} - \frac{1}{2} \right\rangle \quad (14)$$

$$\psi_8 = \left| 31 \frac{1}{2} - \frac{1}{2} \right\rangle = -\sqrt{\frac{2}{3}} |1-1\rangle \left| \frac{1}{2} \frac{1}{2} \right\rangle + \sqrt{\frac{1}{3}} |10\rangle \left| \frac{1}{2} - \frac{1}{2} \right\rangle \quad (15)$$

The matrix elements of H'_{fs} are different, however, as they depend on n and we're using a different value for γ . Since there are only 3 different values of j possible, we can work out the matrix elements of H'_{fs} for these:

$$E_{fs1} \left(j = \frac{1}{2} \right) = -3\gamma \quad (16)$$

$$E_{fs1} \left(j = \frac{3}{2} \right) = -\gamma \quad (17)$$

$$E_{fs1} \left(j = \frac{5}{2} \right) = -\frac{1}{3}\gamma \quad (18)$$

By following the $n = 2$ procedure, we get the upper-left 8×8 block of W :

$$W_{1 \rightarrow 8} = \begin{bmatrix} \beta - 3\gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\beta - 3\gamma & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2\beta - \gamma & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2\beta - \gamma & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{2}{3}\beta - \gamma & -\frac{\sqrt{2}}{3}\beta & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{3}\beta & \frac{1}{3}\beta - 3\gamma & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{2}{3}\beta - \gamma & -\frac{\sqrt{2}}{3}\beta \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{3}\beta & -\frac{1}{3}\beta - 3\gamma \end{bmatrix} \quad (19)$$

To get the lower-right 10×10 block of W , we need to use Clebsch-Gordan coefficients to write the $|nljj_z\rangle$ states in terms of the $|\ell\ell_z\rangle |ss_z\rangle$ states so that we can calculate the matrix elements of H'_Z . We get

$$\psi_9 = \left| 32 \frac{5}{2} \frac{5}{2} \right\rangle = |22\rangle \left| \frac{1}{2} \frac{1}{2} \right\rangle \quad (20)$$

$$\psi_{10} = \left| 32 \frac{5}{2} - \frac{5}{2} \right\rangle = |2-2\rangle \left| \frac{1}{2} - \frac{1}{2} \right\rangle \quad (21)$$

$$\psi_{11} = \left| 32 \frac{5}{2} \frac{3}{2} \right\rangle = \sqrt{\frac{1}{5}} |22\rangle \left| \frac{1}{2} - \frac{1}{2} \right\rangle + \sqrt{\frac{4}{5}} |21\rangle \left| \frac{1}{2} \frac{1}{2} \right\rangle \quad (22)$$

$$\psi_{12} = \left| 32 \frac{3}{2} \frac{3}{2} \right\rangle = \sqrt{\frac{4}{5}} |22\rangle \left| \frac{1}{2} - \frac{1}{2} \right\rangle - \sqrt{\frac{1}{5}} |21\rangle \left| \frac{1}{2} \frac{1}{2} \right\rangle \quad (23)$$

$$\psi_{13} = \left| 32 \frac{5}{2} \frac{1}{2} \right\rangle = \sqrt{\frac{2}{5}} |21\rangle \left| \frac{1}{2} - \frac{1}{2} \right\rangle + \sqrt{\frac{3}{5}} |20\rangle \left| \frac{1}{2} \frac{1}{2} \right\rangle \quad (24)$$

$$\psi_{14} = \left| 32 \frac{3}{2} \frac{1}{2} \right\rangle = \sqrt{\frac{3}{5}} |21\rangle \left| \frac{1}{2} - \frac{1}{2} \right\rangle - \sqrt{\frac{2}{5}} |20\rangle \left| \frac{1}{2} \frac{1}{2} \right\rangle \quad (25)$$

$$\psi_{15} = \left| 32 \frac{5}{2} - \frac{1}{2} \right\rangle = \sqrt{\frac{3}{5}} |20\rangle \left| \frac{1}{2} - \frac{1}{2} \right\rangle + \sqrt{\frac{2}{5}} |2-1\rangle \left| \frac{1}{2} \frac{1}{2} \right\rangle \quad (26)$$

$$\psi_{16} = \left| 32 \frac{3}{2} - \frac{1}{2} \right\rangle = \sqrt{\frac{2}{5}} |20\rangle \left| \frac{1}{2} - \frac{1}{2} \right\rangle - \sqrt{\frac{3}{5}} |2-1\rangle \left| \frac{1}{2} \frac{1}{2} \right\rangle \quad (27)$$

$$\psi_{17} = \left| 32 \frac{5}{2} - \frac{3}{2} \right\rangle = \sqrt{\frac{4}{5}} |2-1\rangle \left| \frac{1}{2} - \frac{1}{2} \right\rangle + \sqrt{\frac{1}{5}} |2-2\rangle \left| \frac{1}{2} \frac{1}{2} \right\rangle \quad (28)$$

$$\psi_{18} = \left| 32 \frac{3}{2} - \frac{3}{2} \right\rangle = \sqrt{\frac{1}{5}} |2-1\rangle \left| \frac{1}{2} - \frac{1}{2} \right\rangle - \sqrt{\frac{4}{5}} |2-2\rangle \left| \frac{1}{2} \frac{1}{2} \right\rangle \quad (29)$$

We can now work out the matrix elements as before to get the bottom-right 10×10 block:

$$W_{9 \rightarrow 18} = \begin{bmatrix} 3\beta - \frac{1}{3}\gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -3\beta - \frac{1}{3}\gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{9}{5}\beta - \frac{1}{3}\gamma & -\frac{2}{5}\beta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{2}{5}\beta & \frac{6}{5}\beta - \gamma & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{3}{5}\beta - \frac{1}{3}\gamma & -\frac{\sqrt{6}}{5}\beta & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{5}\beta & \frac{2}{5}\beta - \gamma & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{3}{5}\beta - \frac{1}{3}\gamma & -\frac{\sqrt{6}}{5}\beta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{5}\beta & -\frac{2}{5}\beta - \gamma & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (30)$$

The energies can now be obtained by finding the eigenvalues of the entire matrix, which isn't that hard since it consists of 6 solo diagonal elements and 6 2×2 blocks. We'll denote the energy corrections by ε_i for $i = 1..18$. The first 4 can be read off the first 4 diagonal entries in $W_{1 \rightarrow 8}$:

$$\varepsilon_1 = \beta - 3\gamma \quad (31)$$

$$\varepsilon_2 = -\beta - 3\gamma \quad (32)$$

$$\varepsilon_3 = 2\beta - \gamma \quad (33)$$

$$\varepsilon_4 = -2\beta - \gamma \quad (34)$$

The next two are the eigenvalues of the sub-matrix $W_{5,6}$:

$$W_{5,6} = \begin{bmatrix} \frac{2}{3}\beta - \gamma & -\frac{\sqrt{2}}{3}\beta \\ -\frac{\sqrt{2}}{3}\beta & \frac{1}{3}\beta - 3\gamma \end{bmatrix} \quad (35)$$

which are:

$$\varepsilon_5 = -2\gamma + \frac{\beta}{2} + \sqrt{\gamma^2 + \frac{\gamma\beta}{3} + \frac{\beta^2}{4}} \quad (36)$$

$$\varepsilon_6 = -2\gamma + \frac{\beta}{2} - \sqrt{\gamma^2 + \frac{\gamma\beta}{3} + \frac{\beta^2}{4}} \quad (37)$$

We can carry on the same way to get the remaining energies:

$$\varepsilon_7 = -2\gamma - \frac{\beta}{2} + \sqrt{\gamma^2 - \frac{\gamma\beta}{3} + \frac{\beta^2}{4}} \quad (38)$$

$$\varepsilon_8 = -2\gamma - \frac{\beta}{2} - \sqrt{\gamma^2 - \frac{\gamma\beta}{3} + \frac{\beta^2}{4}} \quad (39)$$

$$\varepsilon_9 = 3\beta - \frac{1}{3}\gamma \quad (40)$$

$$\varepsilon_{10} = -3\beta - \frac{1}{3}\gamma \quad (41)$$

$$\varepsilon_{11} = -\frac{2}{3}\gamma + \frac{3\beta}{2} + \sqrt{\frac{\gamma^2}{9} + \frac{3\gamma\beta}{5} + \frac{\beta^2}{4}} \quad (42)$$

$$\varepsilon_{12} = -\frac{2}{3}\gamma + \frac{3\beta}{2} - \sqrt{\frac{\gamma^2}{9} + \frac{3\gamma\beta}{5} + \frac{\beta^2}{4}} \quad (43)$$

$$\varepsilon_{13} = -\frac{2}{3}\gamma + \frac{\beta}{2} + \sqrt{\frac{\gamma^2}{9} + \frac{\gamma\beta}{15} + \frac{\beta^2}{4}} \quad (44)$$

$$\varepsilon_{14} = -\frac{2}{3}\gamma + \frac{\beta}{2} - \sqrt{\frac{\gamma^2}{9} + \frac{\gamma\beta}{15} + \frac{\beta^2}{4}} \quad (45)$$

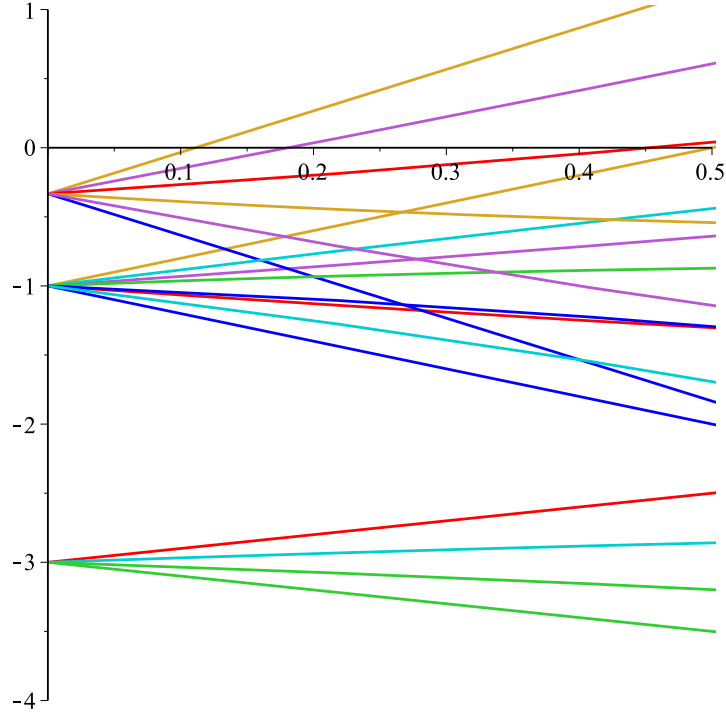
$$\varepsilon_{15} = -\frac{2}{3}\gamma - \frac{\beta}{2} + \sqrt{\frac{\gamma^2}{9} - \frac{\gamma\beta}{15} + \frac{\beta^2}{4}} \quad (46)$$

$$\varepsilon_{16} = -\frac{2}{3}\gamma - \frac{\beta}{2} - \sqrt{\frac{\gamma^2}{9} - \frac{\gamma\beta}{15} + \frac{\beta^2}{4}} \quad (47)$$

$$\varepsilon_{17} = -\frac{2}{3}\gamma - \frac{3\beta}{2} + \sqrt{\frac{\gamma^2}{9} - \frac{3\gamma\beta}{5} + \frac{\beta^2}{4}} \quad (48)$$

$$\varepsilon_{18} = -\frac{2}{3}\gamma - \frac{3\beta}{2} - \sqrt{\frac{\gamma^2}{9} - \frac{3\gamma\beta}{5} + \frac{\beta^2}{4}} \quad (49)$$

Plotting these energies as functions of β gives the following (where $\gamma = 1$):



A closer view shows the weak field case. Note the three distinct starting points for zero field, corresponding to the three values of $j = \frac{5}{2}, \frac{3}{2}, \frac{1}{2}$, reading from the top down.

Finally, we can check that these general results reduce to the weak and strong field values we had earlier. For the weak field case, $\beta \ll \gamma$ and we can expand the expressions for the energies to first order in β to get:

ϵ_1	ϵ_2	ϵ_3	ϵ_4	ϵ_5
$-3\gamma + \beta$	$-3\gamma - \beta$	$-\gamma + 2\beta$	$-\gamma - 2\beta$	$-\gamma + \frac{2}{3}\beta$
ϵ_{10}	ϵ_{11}	ϵ_{12}	ϵ_{13}	ϵ_{14}
$-\frac{1}{3}\gamma - 3\beta$	$-\frac{1}{3}\gamma + \frac{9}{5}\beta$	$-\gamma + \frac{6}{5}\beta$	$-\frac{1}{3}\gamma + \frac{3}{5}\beta$	$-\gamma + \frac{2}{5}\beta$

ϵ_6	ϵ_7	ϵ_8	ϵ_9
$-3\gamma + \frac{1}{3}\beta$	$-\gamma - \frac{2}{3}\beta$	$-3\gamma - \frac{1}{3}\beta$	$-\frac{1}{3}\gamma + 3\beta$
ϵ_{15}	ϵ_{16}	ϵ_{17}	ϵ_{18}
$-\frac{1}{3}\gamma - \frac{3}{5}\beta$	$-\gamma - \frac{2}{5}\beta$	$-\frac{1}{3}\gamma - \frac{9}{5}\beta$	$-\gamma - \frac{6}{5}\beta$

Comparing with the values obtained in the weak field approximation, we find the energies are the same, although they appear in a different order due to the way we labelled the rows in the matrix.

For the strong field limit, $\beta \gg \gamma$ and we get after expanding to first order in γ

ϵ_1	ϵ_2	ϵ_3	ϵ_4	ϵ_5
$-3\gamma + \beta$	$-3\gamma - \beta$	$-\gamma + 2\beta$	$-\gamma - 2\beta$	$-\frac{5}{3}\gamma + \beta$
ϵ_{10}	ϵ_{11}	ϵ_{12}	ϵ_{13}	ϵ_{14}
$-\frac{1}{3}\gamma - 3\beta$	$-\frac{7}{15}\gamma + 2\beta$	$-\frac{13}{15}\gamma + \beta$	$-\frac{3}{5}\gamma + \beta$	$-\frac{11}{15}\gamma$

ϵ_6	ϵ_7	ϵ_8	ϵ_9
$-\frac{7}{3}\gamma$	$-\frac{7}{3}\gamma$	$-\frac{5}{3}\gamma - \beta$	$-\frac{1}{3}\gamma + 3\beta$
ϵ_{15}	ϵ_{16}	ϵ_{17}	ϵ_{18}
$-\frac{11}{15}\gamma$	$-\frac{3}{5}\gamma - \beta$	$-\frac{13}{15}\gamma - \beta$	$-\frac{7}{15}\gamma - 2\beta$

Again, comparing with the strong field approximation, we find that the energies match.