Breit-Rabi formula

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Solution: The purpose is to diagonalize the following matrix,

$$\langle m_I'm_J'|V_{hfs} + V_{zee}(\mathcal{B})|m_Im_J\rangle = \langle m_I'm_J'|\frac{A_J}{\hbar^2}\mathbf{I}\cdot\mathbf{J} + g_J\mu_B\vec{\mathcal{B}}\cdot\mathbf{J} - g_I\mu_N\vec{\mathcal{B}}\cdot\mathbf{I}|m_Im_J\rangle$$
$$= \langle m_I'm_J'|A_J(I_zJ_z + \left(\frac{1}{2}I_+J_- + \frac{1}{2}I_-J_+\right) + g_J\mu_B\mathcal{B}J_z - g_I\mu_N\mathcal{B}I_z|m_Im_J\rangle .$$

Now, since $J = \frac{1}{2}$ we know that there are only two hyperfine states $F = I \pm J = I \pm \frac{1}{2}$. We also know $m_F = m_I + m_J$ and $m_J \pm \frac{1}{2}$. Using the formula,

$$\hat{J}_{\pm}|m_I, m_J\rangle = \hbar \sqrt{J(J+1) - m_J(m_J \pm 1)}|m_I, m_J \pm 1\rangle$$
,

we find,

$$\hat{J}_{\pm}|m_{I}, \pm \frac{1}{2} = 0$$
 and $\hat{J}_{\pm}|m_{I}, \mp \frac{1}{2}\rangle = |m_{I}, \mp \frac{1}{2}\rangle$.

With this, we can calculate the components of the matrix:

$$\begin{split} \langle m_I', \tfrac{1}{2} | V_{hfs} + V_{zee}(B) | m_I, \tfrac{1}{2} \rangle &= (A_J m_I \tfrac{1}{2} + \hbar g_J \mu_B \mathcal{B} \tfrac{1}{2} - \hbar g_I \mu_N \mathcal{B} m_I) \delta_{m_I' m_I} \\ &= \left[\tfrac{A_J}{2} (m_F - \tfrac{1}{2}) + \tfrac{\hbar}{2} (g_J \mu_B - g_I \mu_N) \mathcal{B} - \hbar g_I \mu_N \mathcal{B} m_F \right] \delta_{m_I' m_I} \\ \langle m_I', -\tfrac{1}{2} | V_{hfs} + V_{zee}(B) | m_I, -\tfrac{1}{2} \rangle &= (-A_J m_I \tfrac{1}{2} - \hbar g_J \mu_B \mathcal{B} \tfrac{1}{2} - \hbar g_I \mu_N \mathcal{B} m_I) \delta_{m_I' m_I} \\ &= \left[-\tfrac{A_J^2}{2} (m_F + \tfrac{1}{2}) - \tfrac{\hbar}{2} (g_J \mu_B - g_I \mu_N) \mathcal{B} - \hbar g_I \mu_N \mathcal{B} m_F \right] \delta_{m_I' m_I} \\ \langle m_I', \tfrac{1}{2} | V_{hfs} + V_{zee}(\mathcal{B}) | m_I, -\tfrac{1}{2} \rangle &= \tfrac{A_J}{2} \sqrt{I(I+1) + m_I(m_I-1)} \delta_{m_I' m_I-1} \\ &= \tfrac{A_J}{2} \sqrt{I(I+1) + (m_F^2 - \tfrac{1}{4})} \delta_{m_I' m_I-1} \\ \langle m_I', -\tfrac{1}{2} | V_{hfs} + V_{zee}(\mathcal{B}) | m_I, \tfrac{1}{2} \rangle &= \tfrac{A_J}{2} \sqrt{I(I+1) + m_I(m_I+1)} \delta_{m_I' m_I+1} \\ &= \tfrac{A_J}{2} \sqrt{I(I+1) + (m_F^2 - \tfrac{1}{4})} \delta_{m_I' m_I+1} \; . \end{split}$$

The eigenvalues of this 2×2 matrix are,

$$\Delta E_{hfs} + \Delta E_{zee}(\mathcal{B}) = -\frac{A_J}{4} - g_I \mu_N \mathcal{B} m_F \pm \frac{A_J}{4} \sqrt{-1 + 8 m_F^2 + 4 A_J^2 I(I+1) + 4 m_F x + x^2} \ ,$$

with the abbreviation $x \equiv \frac{2(\mu_B g_J - \mu_N g_I)\mathcal{B}}{A_J}$. This is the Breit-Rabi formula. Note that the derivation can also be made in the base $|(I,J),F,m_F\rangle$ using the formula $\mathbf{I} \cdot \mathbf{J} = \frac{1}{2}(\mathbf{F}^2 - \mathbf{J}^2 - \mathbf{I}^2)$.