VII. Atom in a static magnetic field

What are the good quantum numbers?

$$\hat{H} = -\hat{\vec{\mu}} B + \hat{H}_{hfs}$$

$$\vec{\mu} = g_J \mu_B \hat{\vec{J}} + g_I \mu_N \hat{\vec{I}}$$

We choose axis z along $\vec{B}$.

Then only states with $M_F' = M_F$ are coupled by $\hat{H}$.

$$\langle J I F' M_F | \hat{H} | J I F M_F \rangle =$$

$$= (-B) \frac{C^{F' M_F}_{F M_F 1 0}}{\sqrt{2F'+1}} \left(g_J \mu_B \langle J I F' \| \hat{J}_1 \| J I F \rangle + g_I \mu_N \langle J I F' \| \hat{I}_1 \| J I F \rangle \right) + E_{hfs} \delta_{FF'}$$

$$\langle J I F' \| J_1 \| J I F \rangle =$$

$$= (-1)^{F+J+I+1} \sqrt{(2F'+1)(2F+1)} \times$$

$$\times \begin{Bmatrix} I & J & F \\ 1 & F' & J \end{Bmatrix} \langle J \| \hat{J}_1 \| J \rangle$$

$$\langle J \| \hat{J}_1 \| J \rangle = \sqrt{J(J+1)(2J+1)}$$

$$\langle J I F' \| \hat{I}_1 \| J I F \rangle =$$

$$= (-1)^{F+J+I+1} \sqrt{(2F'+1)(2F+1)}$$

$$\begin{Bmatrix} J & I & F \\ 1 & F' & I \end{Bmatrix} \langle I \| \hat{I}_1 \| I \rangle$$

$$\langle I \| \hat{I}_1 \| I \rangle = \sqrt{I(I+1)(2I+1)}$$

$$E_{hfs} = \frac{A_{hfs}}{2} \left[F(F+1) - J(J+1) - I(I+1) \right]$$

Perform calculations for $J = 1/2$.

$F = I - 1/2$, $F' = I + 1/2$

$(I \geq 1/2)$

The hyperfine energy of the $F = I - 1/2$ state is set to zero.

$$\Delta E_{hfs} = \frac{A_{hfs}}{2} \left[F'(F'+1) - F(F+1) \right] = A_{hfs} (I + 1/2)$$

Diagonal elements of $\hat{H}$

$$\langle J I F M_F | \hat{H} | J I F M_F \rangle = \delta_{F\, I+1/2} \Delta E_{hfs} + $$

$$+ E_{M_F}(F)$$

$$E_{M_F}(F) = -B \frac{C^{F M_F}_{F M_F 1 0}}{\sqrt{2F+1}} \times (-1)^{\frac{1}{2}+I+F+1} \times$$

$$\times \sqrt{(2F+1)(2F+1)} \left(g_J \mu_B \begin{Bmatrix} I & 1/2 & F \\ 1 & F & 1/2 \end{Bmatrix} \sqrt{\tfrac{1}{2}\cdot\tfrac{3}{2}\cdot 2} + \right.$$

$$\left. + g_I \mu_N \begin{Bmatrix} 1/2 & I & F \\ 1 & F & I \end{Bmatrix} \sqrt{I(I+1)(2I+1)} \right)$$

$$C^{F M_F}_{F M_F 1 0} = \frac{M_F}{\sqrt{F(F+1)}}$$

$$\begin{Bmatrix} I & 1/2 & F \\ 1 & F & 1/2 \end{Bmatrix} = \frac{(-1)^{\frac{1}{2}+I+F+1}}{2} \times$$

$$\times \frac{F(F+1) - I(I+1) + \frac{1}{2}\cdot\frac{3}{2}}{\sqrt{F(F+1)(2F+1)\cdot\frac{1}{2}\cdot\frac{3}{2}\cdot 2}}$$

$$\begin{Bmatrix} 1/2 & I & F \\ 1 & F & I \end{Bmatrix} = \frac{(-1)^{1/2+I+F+1}}{2} \frac{F(F+1) + I(I+1) - \frac{1}{2}\frac{3}{2}}{\sqrt{F(F+1)(2F+1)\, I(I+1)(2I+1)}}$$

$$E_{M_F}(F) = -B M_F \left(g_J \mu_B \frac{F(F+1) - I(I+1) + \frac{3}{4}}{2F(F+1)} + \right.$$

$$\left. + g_I \mu_N \frac{F(F+1) + I(I+1) - 3/4}{2F(F+1)} \right)$$

$$\mu_B = 9{,}27 \cdot 10^{-24} \ \frac{J}{T}$$

$$h = 2\pi\hbar = 6.63 \cdot 10^{-34} \ J \cdot s$$

$$\frac{\mu_B}{2\pi\hbar} = 1{,}4 \cdot 10^{10} \ \frac{Hz}{T} = 1{,}4 \cdot 10^{4} \ \frac{MHz}{T} =$$

$$= 1{,}4 \ \frac{MHz}{G} \qquad (CGS)$$

$$g_J = -\left(1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} \right)$$

Ground state of an alkali atom:

$$L = 0 \qquad S = 1/2 \qquad J = 1/2$$

$$g_{J=1/2} = -2$$

$F = I \pm \frac{1}{2}$:

$$\frac{F(F+1) - I(I+1) + \frac{3}{4}}{2F(F+1)} = \pm \frac{1}{1+2I}$$

^{87}Rb : $I = 3/2$, $\frac{1}{1+2I} = \frac{1}{4}$

In weak fields ($E_z(F) \ll \Delta E_{hfs}$) we have **for ^{87}Rb**

$$E_{M_F}(F = I \pm 1/2) = -0{,}7\ \frac{\text{MHz}}{\text{T}}\, 2\pi\hbar\, B\, M_F$$

Nuclear spin contribution is small

$$\frac{F(F+1) + I(I+1) - \frac{3}{4}}{2F(F+1)} = \begin{cases} \dfrac{2(I+1)}{2I+1}, & F = I - \frac{1}{2} \\[2ex] \dfrac{2I}{2I+1}, & F = I + \frac{1}{2} \end{cases}$$

For ^{87}Rb

$g_I = 1{,}833$ ← Nuclear-physics definition

$\tilde{g}_I = \dfrac{g_I \mu_N}{\mu_B} \simeq 1 \cdot 10^{-3}$ ← Often used in spectroscopy

$E_{M_F} = \pm(I + 1/2)$ ($F = I + 1/2$) yields the exact energy

Weak-field limit

($\mu_B B \ll \Delta E_{hfs}$) , $\Delta E_{hfs} > 0$ (^{87}Rb)

$$E_+ \approx \Delta E_{hfs} + E_{M_F}(I + 1/2) + \frac{H_\perp^2(M_F)}{\Delta E_{hfs}}$$

$$E_- \approx E_{M_F}(I - 1/2) - \frac{H_\perp^2(M_F)}{\Delta E_{hfs}}$$

Opposite (strong-field) limit

$$\begin{aligned} E_\pm \approx\ & \frac{1}{2}\left[E_{M_F}(I+1/2) + E_{M_F}(I-1/2)\right] \pm \\ & \pm \sqrt{\frac{1}{4}\left[E_{M_F}(I+1/2) - E_{M_F}(I-1/2)\right]^2 + H_\perp^2(M_F)} + \\ & + \frac{\Delta E_{hfs}}{2} \pm \frac{\Delta E_{hfs}\left(E_{M_F}(I+1/2) - E_{M_F}(I-1/2)\right)}{4\sqrt{\frac{1}{4}\left[E_{M_F}(I+1/2) - E_{M_F}(I-1/2)\right]^2 + H_\perp^2(M_F)}} \end{aligned}$$

Terms:

Independent of B

Linear in B

Quadratic in B

Off-diagonal matrix element for states with $|M_F| \neq I + \frac{1}{2}$

$$H_\perp(M_F) = \langle J = 1/2 \; I \; F' = I + \tfrac{1}{2} \; M_F | \hat{H} | J = 1/2 \; I \; F = I - 1/2 \; M_F \rangle$$

$$\hat{H} = \begin{pmatrix} \Delta E_{hfs} + E_{M_F}(I+1/2) & H_\perp(M_F) \\ H_\perp(M_F) & E_{M_F}(I-1/2) \end{pmatrix}$$

Breit-Rabi Formula for the eigenenergies

$$\boxed{E_\pm = \frac{1}{2}\left[\Delta E_{hfs} + E_{M_F}(I+1/2) + E_{M_F}(I-1/2)\right] \pm \sqrt{\frac{1}{4}\left[\Delta E_{hfs} + E_{M_F}(I+1/2) - E_{M_F}(I-1/2)\right]^2 + H_\perp^2(M_F)}}$$

$$\Delta E_{hfs} \propto B^0 \equiv \text{const}$$

$$E_{M_F}(I \pm 1/2), \; H_\perp(M_F) \propto B$$

Explicitly for $J = 1/2$ and $|M_F| \neq I + 1/2$

$$H_\perp(M_F) = \langle \tfrac{1}{2}\, I\, F' = I+\tfrac{1}{2}\, M_F \,|\, (-B)(g_J \mu_B \hat{J}_z +$$

$$+ g_I \mu_N \hat{I}_z) \,|\, \tfrac{1}{2}\, I\, F = I - 1/2\;\, M_F \rangle$$

$\hat{F}_z = \hat{J}_z + \hat{I}_z$ does not couple states with $F' \neq F$

$$H_\perp(M_F) = B(g_J \mu_B - g_I \mu_N) \times$$

$$\times \langle \tfrac{1}{2}\, I\, F' = I + \tfrac{1}{2}\, M_F \,|\, \hat{I}_{10} \,|\, \tfrac{1}{2}\, I\, F = I - \tfrac{1}{2}\, M_F \rangle =$$

$$= B(g_J \mu_B - g_I \mu_N)\, C^{I+\frac{1}{2}\;\, M_F}_{I-\frac{1}{2}\;\, M_F\; 10} \sqrt{2(I-\tfrac{1}{2})+1} \times$$

$$\times (-1)^{I-\frac{1}{2}+\frac{1}{2}+I+1} \begin{Bmatrix} \frac{1}{2} & I & I-\frac{1}{2} \\ 1 & I+\frac{1}{2} & I \end{Bmatrix} \sqrt{I(I+1)(2I+1)}$$

$$\begin{Bmatrix} \frac{1}{2} & I & I-\frac{1}{2} \\ 1 & I+\frac{1}{2} & I \end{Bmatrix} = \begin{Bmatrix} 1 & I & I \\ \frac{1}{2} & I-\frac{1}{2} & I+\frac{1}{2} \end{Bmatrix} =$$

$$= (-1)^{2I+1} \cdot \frac{1}{2} \sqrt{\frac{2}{(2I+1)^2 \, I(I+1)}}$$

$$C^{I+\frac{1}{2}\, M_F}_{I-\frac{1}{2}\, M_F\, 10} = \sqrt{\frac{(I+\frac{1}{2}+M_F)(I+\frac{1}{2}-M_F)}{2I(I+\frac{1}{2})}}$$

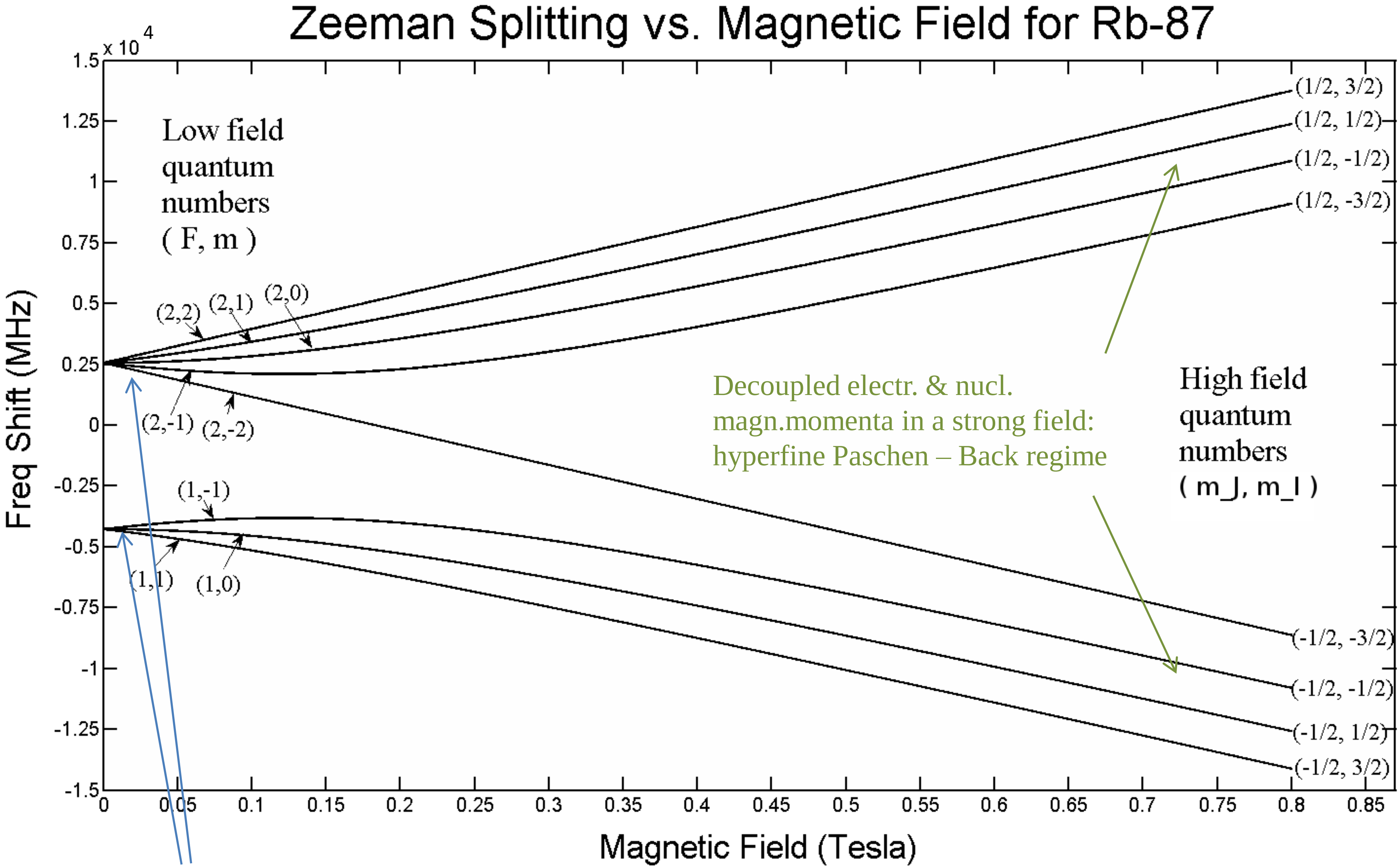
$$H_\perp(M_F) = \frac{\sqrt{(I+\frac{1}{2})^2 - M_F^2}}{2I+1} \cdot B(g_J \mu_B - g_I \mu_N)$$

$$E_{M_F}(I+\tfrac{1}{2}) - E_{M_F}(I-\tfrac{1}{2}) = -\frac{2M_F}{2I+1} B(g_J \mu_B - g_I \mu_N)$$

$$E_{M_F}(I+\tfrac{1}{2}) + E_{M_F}(I-\tfrac{1}{2}) = -2M_F \, B g_I \mu_N$$

$$E_\pm \simeq -\left[\mp \frac{1}{2} g_J \mu_B B + g_I \mu_N B \left(M_F \pm \frac{1}{2}\right)\right]$$

In the leading order the energy of decoupled electr. momentum with $J_z = \mp\frac{1}{2}$ and nucl. spin with $I_z = M_F \pm \frac{1}{2}$



Zeeman effect in a small magn.field

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