The Zeeman Effect

(& Atoms in static fields)

So far, we've only considered "bare" atomic structure, i.e. the problem of isolated atoms in the absence of applied fields.

We described important parts of this structure, namely the spin-orbit part of the fine structure and the hyperfine interactions as electron spins and nuclear spins interacting w/ an effective B-field, i.e.

Fine structure	Hyperfine
$H_{s\text{-}o} = -\vec{\mu}_{el} \cdot \vec{B}_{eff}$	$H_{hfs} = -\vec{\mu}_{I} \cdot \vec{B}_{eff}$
$H_{s\text{-}o} \propto \vec{S} \cdot \vec{L}$	$H_{hfs} \propto \vec{I} \cdot \vec{J}$

It's natural to ask, "what effect does an external (static) magnetic field have on our states and their energies?"

General picture:

We've seen that the various angular momenta get "coupled" by their interactions, such that the symmetry of the Hamiltonian is changed and new quantum numbers / basis states are relevant

i.e. for $\vec{S}\cdot\vec{L}$, $|J, m_J\rangle$ instead of $|m_L, m_S\rangle$

and for $\vec{I}\cdot\vec{J}$, $|F, m_F\rangle$ instead of $|m_I, m_J\rangle$

When the change in energy due to the applied field begins to dominate over the contribution due to these ($\vec{S}\cdot\vec{L}$, $\vec{I}\cdot\vec{J}$) interactions, the angular momenta will ~~beg~~ become uncoupled (decoupled), and the states w/ well-defined angular momentum w/ respect to the z-axis (direction of applied field, breaking symmetry of the problem) for the respective components will become our good ~~eigenstates~~ basis states.

③ Let's start by neglecting hyperfine (think $I=0$)

new term in Hamiltonian given by

see Foot Ch 5.5

$$\mathcal{H}_B = -\vec{\mu} \cdot \vec{B}_{ext}$$

assume $\vec{B}_{ext} = B_z \hat{z}$

where

$$\vec{\mu} = \vec{\mu}_e + \vec{\mu}_s$$

due to electron spin angular momentum

due to electron orbital angular momentum

$$\vec{\mu}_e = -\frac{\mu_B}{\hbar} \vec{L} \quad \text{and} \quad \vec{\mu}_s = -g_s \frac{\mu_B}{\hbar} \vec{S}$$

recall Gabrielse colloquium

$g_s \approx 2$ for electron spin

in general, g-factors just help us relate magnetic moment $\vec{\mu}$ w/ some generic spin $\vec{J}, \vec{I}$, e

for low fields, $E_{zeeman} \sim \mu_B B_z << E_{s-o}$ (ΔE_{fs} in general),

J, m_J will remain good quantum numbers, i.e. $\vec{L}$ and $\vec{S}$ will still be coupled as their interactions are the dominant term.

→ rewrite as $\mathcal{H}_B = \frac{\mu_B}{\hbar} g_J \vec{J} \cdot \vec{B}_{ext}$ where $g_J \vec{J} = \vec{L} + g_s \vec{S}$

The Landé g-factor g_J can be found at low field by considering the projection of $\vec{\mu}$ onto $\vec{J}$

w/ projection theorem:

$$\langle J, m_J' | \vec{X} | J, m \rangle = \frac{\langle \vec{J} \cdot \vec{X} \rangle}{J(J+1)\hbar^2} \langle J, m' | \vec{J}$$

$$g_J = \frac{\langle \vec{L} \cdot \vec{J} \rangle + g_s \langle \vec{S} \cdot \vec{J} \rangle}{J(J+1)\hbar^2}$$

w/ $g_s \simeq 2$

$$g_J = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)} = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}$$

The 1st order energy shift at low fields will be

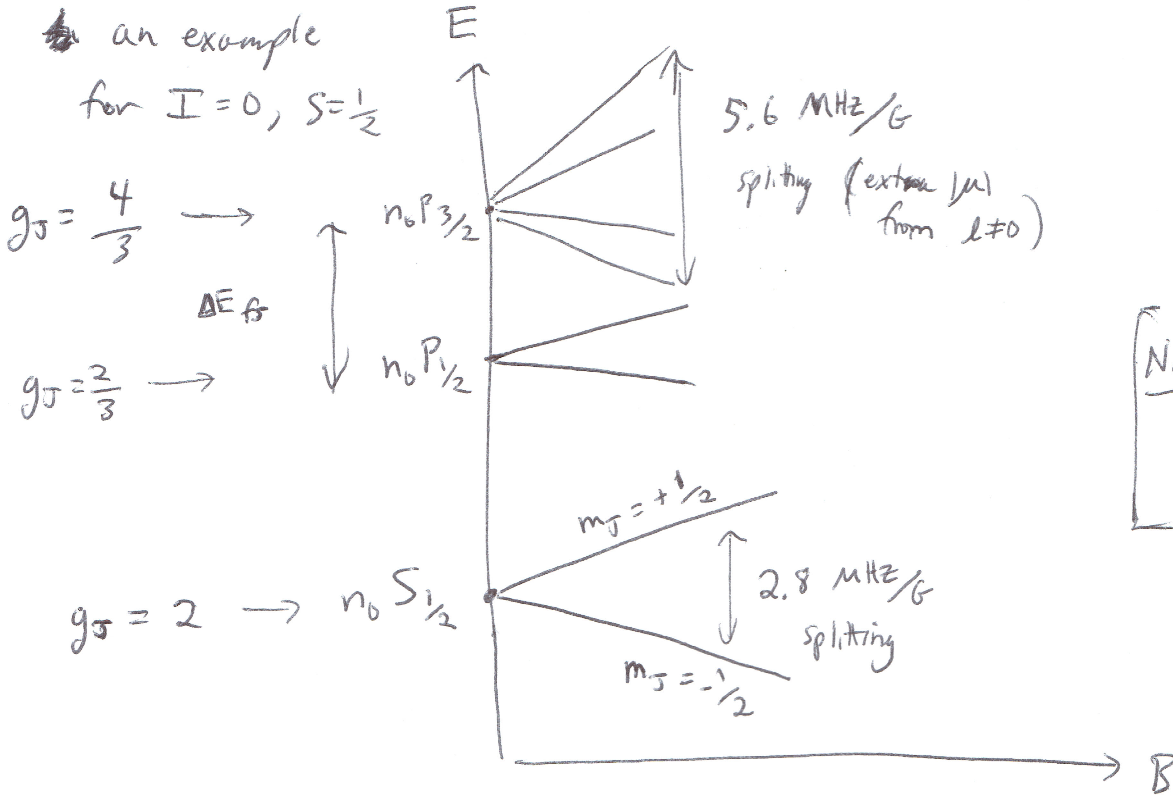
$$\Delta E = \langle n, J, m_J | \mathcal{H}_B | n, J, m_J \rangle = \frac{\mu_B}{\hbar} g_J \langle n, J, m_J | \vec{J} \cdot \vec{B} | n, J, m_J \rangle$$

w/ $\vec{B} = B_z \hat{z}$

$$\Delta E = \frac{\mu_B}{\hbar} g_J \langle n, J, m_J | J_z | n, J, m_J \rangle = \mu_B g_J m_J B_z$$

~ linear shift in energy according to m_J, g_J values

an example for $I = 0$, $S = \frac{1}{2}$



Note: in H,
for the excited, $n_0 = 2$ st
$E_{S_{1/2}} > E_{P_{1/2}}$

again, this low-field, ~linear Zeeman shift regime will basically hold as long as $E_{Zeeman} \sim \mu_B B_z \ll \Delta E_{fs}$

for H, $\Delta E_{fs} \sim 10$ GHz, $\mu_B \approx 1.4$ MHz/G

expect around $\approx 1T = 10{,}000$ G for this to break down completely

for heavy alkalis, more like $10^2 - 10^4$ T

(5) High-field limit $\mu_B B_z \gg \Delta E_{fs}$

In this limit, m_L and m_S are the "good" quantum numbers (states w/ well-defined ang. mom. w.r.t. the z-axis for both $\vec{L}$ & $\vec{S}$), and spin-orbit coupling is only a perturbation

This is referred to as the Paschen-Back limit

$$H = \frac{\mu_B}{\hbar}(\vec{L} + g_s\vec{S})\cdot\vec{B} = \frac{\mu_B}{\hbar}(\vec{L} + 2\vec{S})\cdot\vec{B}$$

and the Zeeman component of the energy is

$$E_{mag} = \langle n, L, S, m_L, m_S | H | n, L, S, m_L, m_S \rangle = \mu_B B(m_L + 2m_S)$$

for hydrogen we'll find this limit for

$\mu_B B \gg \Delta E_{fs}$, $B \sim 10T$

<u>Li</u> $\rightarrow \Delta E_{fs} \approx 10$ GHz, so roughly same as H

for heavier <u>alkalis</u>, $\Delta E_{fs} \sim 0.5$ THz for Na

~ 2 THz for K

~ 7 THz for Rb

~ 16 THz for Cs

$\rightarrow$ need fields of roughly $10^2 - 10^4$ T

or $10^6 - 10^8$ G

hard to get to Paschen-Back regime for fine structure

<u>Let's look @ hyperfine structure</u>

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Zeeman w/ hyperfine structure

the interactions of the various angular momentum components w/ an external field can again be written as

$$H = -\vec{\mu} \cdot \vec{B}_{ext}$$

where

$$\vec{\mu} = \vec{\mu}_L + \vec{\mu}_S + \vec{\mu}_I$$

$$\vec{\mu} = -\frac{\mu_B}{\hbar}(\vec{L} + g_S \vec{S}) + \vec{\mu}_I$$

we saw that the expression for $\vec{\mu}_I$ varies quite a bit from reference to reference. ~~Both~~ ~~Both~~ Both the sign and magnitude convention for g_I ~~change~~ vary

e.g. $\mu_I = +\frac{g_I \mu_N}{\hbar}\vec{I}$ is sometimes used, where $\mu_N = \mu_B \frac{m_e}{m_p} \approx \frac{\mu_B}{1836}$ and g_I is of order unity

or $\mu_I = +\frac{g_I \mu_B}{\hbar}\vec{I}$ is also used, where g_I is of order ~~as~~ 10^{-3}

<u>Note</u>: conventions w/ the opposite <u>sign are also used</u>

(watch signs / magnitudes on HW question - be consistent w/ Steck)

⑦

We'll write

$$H = \frac{\mu_B}{\hbar}(\vec{L} + g_s\vec{S}) - \frac{g_I \mu_N}{\hbar}\vec{I},$$

where $g_s \simeq 2$ and g_I is of order unity, depending on the atom's nuclear state

Again, we saw that F & m_F were good quantum numbers in zero B-field, where the $\vec{I}\cdot\vec{J}$ interaction was the dominant perturbation to H_{FS}.

<u>Low-field limit</u> $\mu_B B << \Delta E_{hfs}$

F & m_F will remain good quantum #'s in this limit.

$$H_B^{low} \approx \frac{\mu_B}{\hbar} g_F \vec{F}\cdot\vec{B}$$

comes from projecting $\vec{J}$ onto $\vec{F}$

where $$g_F = g_J \frac{F(F+1) - I(I+1) + J(J+1)}{2F(F+1)}$$

from projecting $\vec{I}$ onto $\vec{F}$

$$+ \, g_I \frac{\mu_N}{\mu_B} \frac{F(F+1) - J(J+1) + I(I+1)}{2F(F+1)}$$

smaller by roughly 10^{-3} factor

$$g_F \approx g_J \frac{F(F+1) - I(I+1) + J(J+1)}{2F(F+1)}$$

⑧

$$\Delta E^{\text{low-field}}_{\text{zeeman}} = \langle H_B^{\text{low}} \rangle = \langle F, m_F | \frac{\mu_B}{\hbar} g_F \vec{F} \cdot \vec{B} | F, m_F \rangle$$

$$= \mu_B g_F m_F B_z$$

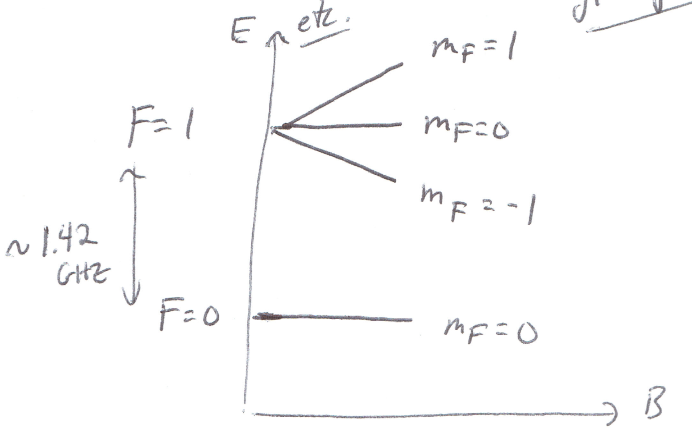
, where we assume $\vec{B} = B_z \hat{z}$ w.l.o.g.

$\boxed{\text{for low fields}}$

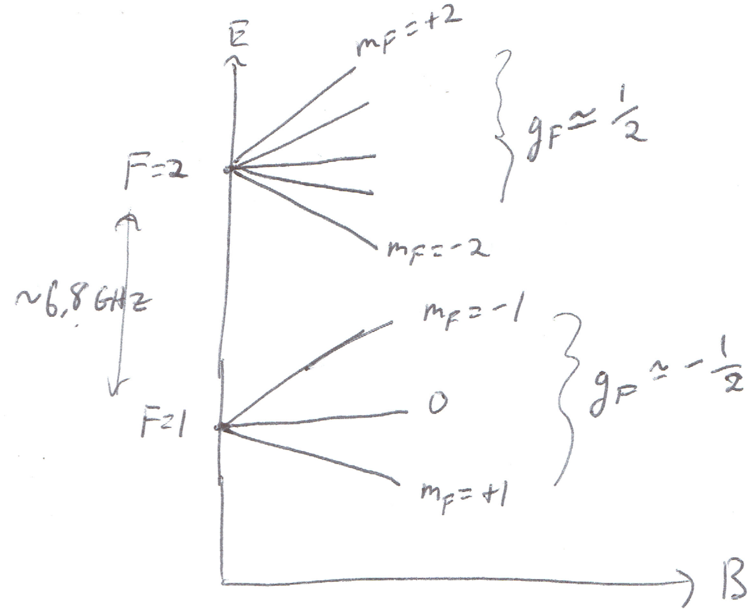
as before

$g_F \approx g_J = 2$

for ^{87}Rb, $I = 3/2$



as in hydrogen, $I = \frac{1}{2}$ for $1S_{1/2}$



At high fields, where high means $\Delta E_{\text{zeeman}} \sim \mu_B B_z \gg \Delta E_{hfs}$,

Back-Goudsmit regime (also called Paschen-Back)

$\vec{I}$ and $\vec{J}$ are uncoupled, and states w/ well-defined ang. mom. w.r.t. $\hat{z}$ are again the good eigenstates,

so $|F, m_F\rangle \rightarrow |m_I, m_J\rangle$

at high fields, the hyperfine ($\vec{I} \cdot \vec{J}$) interaction is just a perturbat[ion] that gets less important as B_z increases.

(9)

$$H_B^{high} = \left[\frac{\mu_B}{\hbar}(\vec{L} + g_s \vec{S}) - \frac{g_I \mu_N}{\hbar} \vec{I}\right] \cdot \vec{B}$$

$$\Delta E_B^{high} = \langle I, m_I, J, m_J | H_B^{high} | I, m_I, J, m_J \rangle \qquad \text{w/ } \vec{B} = B_z \hat{z}$$

$$= \mu_B \left[g_J m_J - g_I \frac{\mu_N}{\mu_B} m_I \right] B_z$$

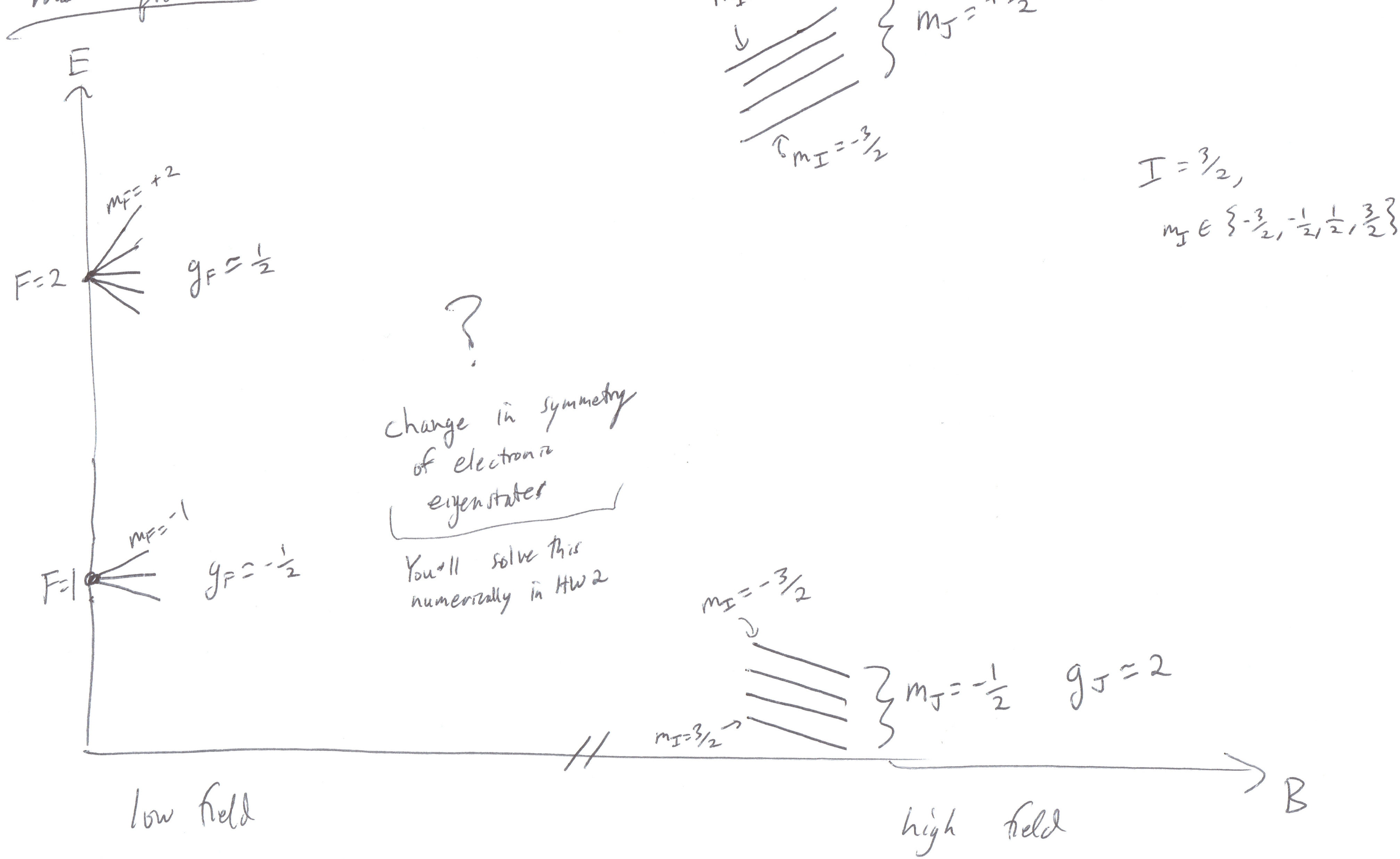
at which field this occurs, i.e. when the linear Zeeman effect fully breaks down, depends on the atom (i.e. on A_{hfs}) as well on whether you're considering the s-levels or excited states.

Typical value, for $A \sim 1\,\text{GHz}$ and $\mu_B = 1.4\ \frac{\text{MHz}}{\text{G}}$, will be roughly 100s of gauss

The $\vec{I} \cdot \vec{J}$ coupling will still have an absolute energy shift at high fields, w/

$$\Delta E_{IJ}^{high} = \langle I, m_I, J, m_J | h A_{hfs} \frac{\vec{I} \cdot \vec{J}}{\hbar^2} | I, m_I, J, m_J \rangle = h A_{hfs} m_I m_J$$

Whole picture (for ^{87}Rb, $I = 3/2$)



$\boxed{\text{Major note}}$ $\mu = -\frac{\partial E}{\partial B}$, i.e. the slope of the energy on this ... magnetic moment ... depends on B

$$\mathcal{H} = h A_{hfs} \frac{\vec{I}\cdot\vec{J}}{\hbar^2} \underbrace{- \vec{\mu}_J \cdot \vec{B} - \vec{\mu}_I \cdot \vec{B}}$$

diagonal in $|F, m_F\rangle$ basis

diagonal in $|m_I, m_J\rangle$ basis

w/ $\vec{B}$ along $\hat{z}$, express as

$$\mathcal{H} = h A_{hfs} \frac{\vec{I}\cdot\vec{J}}{\hbar^2} + \frac{\mu_B}{\hbar}\left[g_J J_z - g_I \frac{\mu_N}{\mu_B} I_z \right] B_z$$

need to express in terms of $|I, m_I, J, m_J\rangle$ states

~~Clebsch-Gordan coefficients~~

in HW#2, you'll write down $\mathcal{H}$ as a matrix and diagonalize it, solving for eigenstates and energies

For the particular case of alkali ground states, there's an analytical solution (Breit-Rabi formula)

$\boxed{L=0}$ so $\vec{J} = \vec{S}$ and $\vec{I}\cdot\vec{J} = \vec{I}\cdot\vec{S} = \sum_{\sigma \in (x,y,z)} I_\sigma S_\sigma = I_z J_z + \frac{1}{2}(I_+ S_- + I_- S_+)$

diagonal

off-diagonal

Key task, just constructing $\langle m_I', m_J' | \frac{I_+ S_- + I_- S_+}{2} | m_I, m_J\rangle$ terms, then solve

The solution, the Breit-Rabi formula, is

$$E = \frac{-\Delta E_{hfs}}{2(2I+1)} - g_I \mu_N m B_z \pm \frac{\Delta E_{hfs}}{2}\sqrt{1 + \frac{4mX}{2I+1} + X^2}$$

where $m = m_I \pm m_J$ depending on this sign,

$$X = \frac{\left(g_J + g_I \frac{\mu_N}{\mu_B}\right)}{\Delta E_{hfs}} \mu_B B_z$$

and $\Delta E_{hfs} = \frac{(2I+1)hA}{2}$

also $\underbrace{|F, m_F\rangle}$ $= \alpha(B_z)\,|m_I = m_F - \frac{1}{2}, m_s = \frac{1}{2}\rangle$

$+ \beta(B_z)\,|m_I = m_F + \frac{1}{2}, m_s = -\frac{1}{2}\rangle$

labeling state by the zero-field state to which it connects

change of α, β w/ B_z relates to change of symmetry, change of eigenstates