PHY 446 3/23/2020

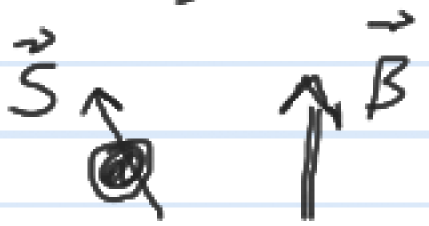
ATOMS IN MAGNETIC FIELDS

APPLICATIONS:

- CHEMISTRY (NMR)
- MEDICINE (MRI)
- MAGNETIC TRAPPING OF COLD ATOMS
  - MAGNETO-OPTICAL TRAP (MOT)
- ASTROPHYSICS

WARM-UP: ELECTRON SPIN IN $\vec{B}$-FIELD

ELECTRON $S = 1/2$, $\vec{B} = B\hat{z}$



FIND ENERGY LEVELS

$$H = -\vec{\mu}_s \cdot \vec{B}$$

$$\vec{\mu}_s = -g_s \mu_B \vec{S}/\hbar$$

$\leftarrow$ ELECTRON SPIN g FACTOR

$g_s \approx 2.0$

$$E = \frac{2\mu_B}{\hbar} \vec{B} \cdot \vec{S} \checkmark$$

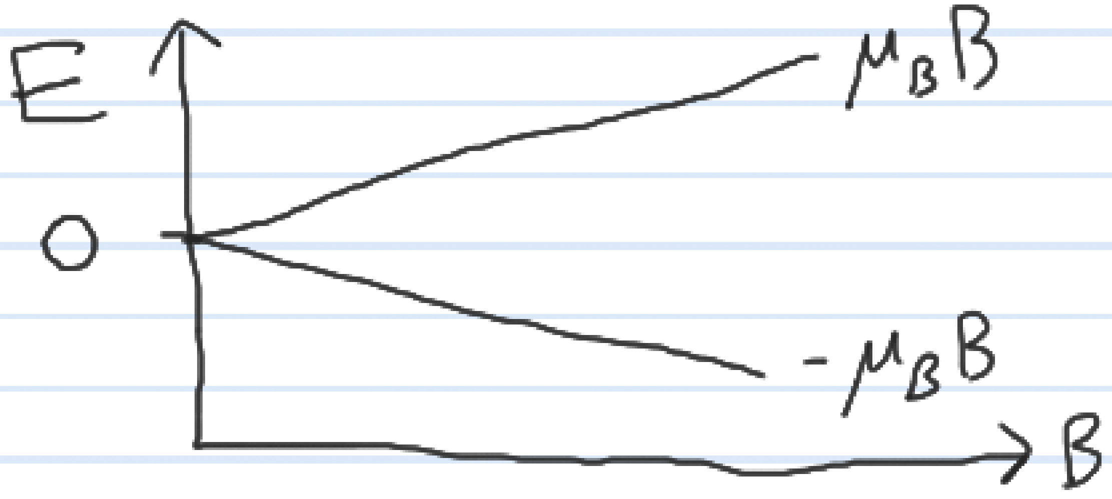
$$H = g_s \mu_B \vec{S} \cdot \vec{B}/\hbar = g_s \mu_B S_z B/\hbar$$

ENERGY

STATE $|m_s\rangle$, $m_s = \pm\frac{1}{2}$

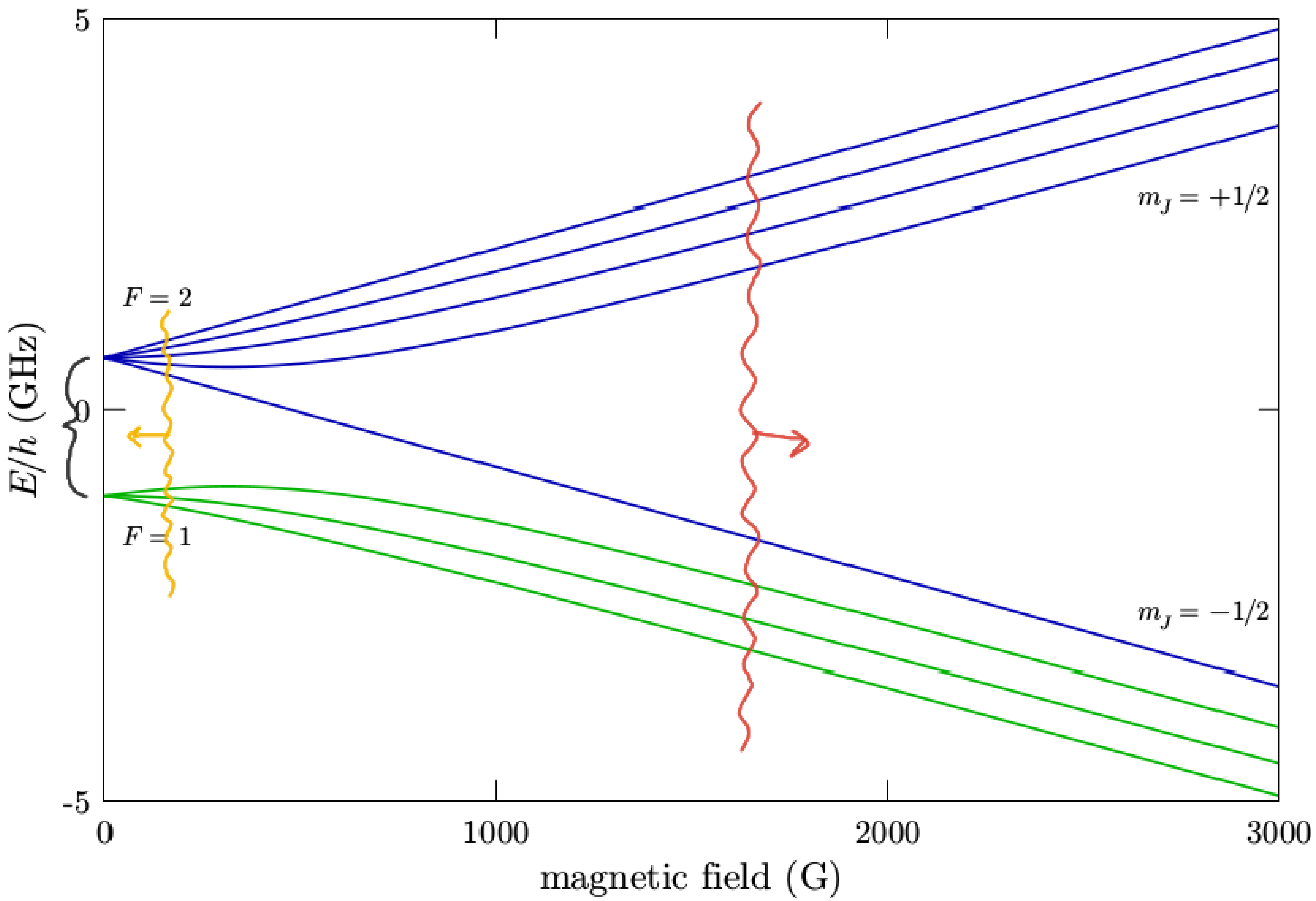
$$E = \langle m_s|H|m_s\rangle = \langle m_s|\, \mu_B g_s B S_z/\hbar\,|m_s\rangle = \frac{\mu_B g_s B}{\hbar} \underbrace{\langle m_s|S_z|m_s\rangle}_{\hbar m_s}$$

$$= \mu_B g_s B\, m_s \qquad , \quad m_s = \pm\frac{1}{2}$$



^{23}Na GND STATE

$$H_{HFS} = \frac{A\,\vec{I}\cdot\vec{J}}{\hbar^2}$$



ELECTRON SPIN $\vec{S}$

ORBITAL $\vec{L}$

$\vec{J} = \vec{L} + \vec{S}$

NUCLEAR SPIN $\vec{I}$

FINE STRUCTURE: SPIN-ORBIT COUPLING

$$H_{FS} = -\vec{\mu}_S \cdot \vec{B}_L = \beta\, \vec{L}\cdot\vec{S}/\hbar^2$$

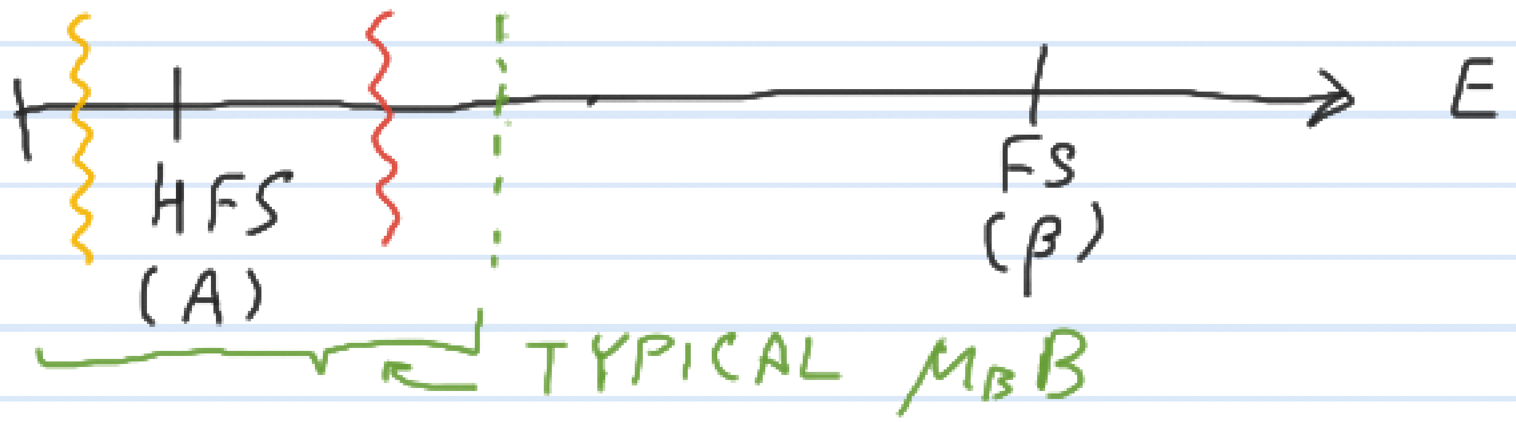
HYPERFINE: NUCLEAR SPIN INTERACTS W/ ELECTRON'S MAGNETIC FIELD

$$H_{HFS} = -\vec{\mu}_I \cdot \vec{B}_J = A\, \vec{I}\cdot\vec{J}/\hbar^2$$

NOW, ADD EXTERNAL $\vec{B}$ FIELD $\vec{B} = B\hat{z}$

$$H' = -(\vec{\mu}_L + \vec{\mu}_S + \vec{\mu}_I)\cdot\vec{B} \approx -(\vec{\mu}_L + \vec{\mu}_S)\cdot\vec{B} \quad \text{b/c} \quad \frac{\mu_N}{\mu_B} = \frac{m_e}{m_p} \sim 5\times 10^{-4}$$

TYPICAL SCALES



FIRST, CONSIDER $HFS \ll \mu_B B \ll FS$

- CAN NEGLECT NUCLEAR SPIN (i.e. HFS)
- H' WEAK PERTURBATION OF H_{FS}

$$H_{FS} = \beta \vec{L} \cdot \vec{S} / \hbar^2 = \frac{\beta}{2\hbar^2}\left(\vec{J}^2 - \vec{L}^2 - \vec{S}^2\right)$$

$$H' = -(\vec{\mu}_L + \vec{\mu}_S) \cdot \vec{B} = \mu_B (g_L \vec{L} + g_S \vec{S}) \cdot \vec{B}/\hbar = \frac{\mu_B B}{\hbar}(g_L L_z + g_S S_z)$$

$g_L \approx 1.0, \quad g_S \approx 2.0$

J_z IS A GOOD QUANTUM NUMBER: $[H, J_z] = [H_{FS} + H', J_z] = 0$

- ROTATIONAL SYMMETRY ABOUT $\hat{z}$

ENERGY SHIFT

$$\Delta E = \langle H' \rangle = \langle J M_J | H' | J M_J \rangle = \frac{\mu_B B}{\hbar} \langle J M_J | g_L L_z + g_S S_z | J M_J \rangle$$

$\langle L_z \rangle = ?$

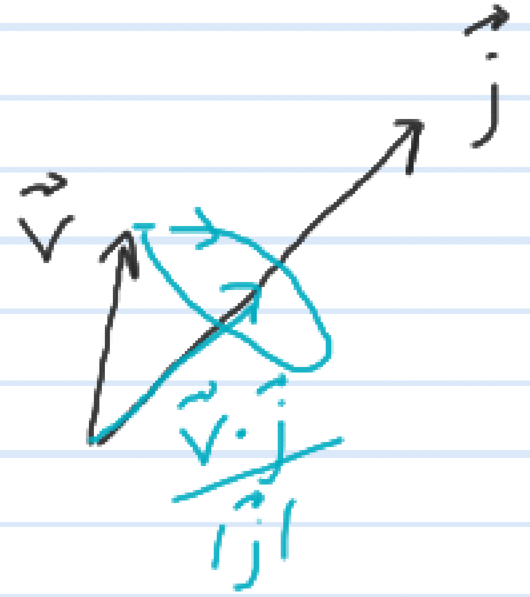
$\langle S_z \rangle = ?$

PROJECTION THEOREM

SYSTEM W/ TOTAL ANG. MOM. $\vec{j}$

ANY VECTOR $\vec{V}$

$$\langle j m_j | V_z | j m_j \rangle = \frac{\langle j m_j | \vec{V}\cdot\vec{j} | j m_j \rangle}{\hbar^2 j(j+1)} \hbar m_j$$



- FORMAL PROOF VIA WIGNER-ECKART THEOREM
- INFORMAL INTERPRETATION: $\vec{V}$ PRECESSES $\vec{j}$

$$\langle \vec{V} \rangle = \vec{V}_{\parallel} = \mathrm{Proj}_{\vec{j}}(\vec{V}) = \frac{\vec{V}\cdot\vec{j}}{|\vec{j}|}\frac{\vec{j}}{|\vec{j}|} = \frac{\vec{V}\cdot\vec{j}}{|\vec{j}|^2}\vec{j}$$

$$\langle V_z \rangle = \langle \vec{V} \rangle \cdot \hat{z} = \frac{\vec{V}\cdot\vec{j}}{|\vec{j}|^2} j_z = \frac{\vec{V}\cdot\vec{j}}{\hbar^2 j(j+1)} \hbar m_j \quad \checkmark$$

APPLY TO $\langle J M_J | L_z | J M_J \rangle$

$\vec{j} \to \vec{J}$, $\vec{V} \to \vec{L}$

$$\Rightarrow \langle J M_J | L_z | J M_J \rangle = \frac{\langle J M_J | \vec{L}\cdot\vec{J} | J M_J \rangle}{\hbar^2 J(J+1)} \hbar M_J$$

3/25/2020

ATOMS IN $\vec{B}$ FIELDS

ELECTRON $\vec{S}, \vec{L}$

NUCLEAR $\vec{I}$

FS: $H_{FS} = \beta \vec{S}\cdot\vec{L}/\hbar^2$

HFS: $H_{HFS} = A\vec{I}\cdot\vec{J}/\hbar^2 \qquad (\vec{J} = \vec{L}+\vec{S})$

CONSIDER: $HFS \ll \mu_B B \ll FS$

$$H' = -(\vec{\mu}_L + \vec{\mu}_S + \cancel{\vec{\mu}_I})\cdot\vec{B} \approx -(\vec{\mu}_L + \vec{\mu}_S)\cdot\vec{B} = \mu_B(g_L\vec{L} + g_S\vec{S})\cdot\vec{B}/\hbar$$

$\vec{B} = B\hat{z}$

• FOOT 5.5

$$H' = \mu_B(g_L L_z + g_S S_z)B/\hbar$$

$$\Delta E = \langle H' \rangle = \frac{\mu_B B}{\hbar}\left(g_L\langle L_z\rangle + g_S\langle S_z\rangle\right)$$

STATE: $|J M_J\rangle$: $\langle L_z\rangle = \langle J M_J | L_z | J M_J\rangle$

PROJECTION THEOREM

$$\langle JM_J|L_z|JM_J\rangle = \frac{\langle JM_J|\vec{L}\cdot\vec{J}|JM_J\rangle}{\hbar^2 J(J+1)}\hbar M_J$$

EVALUATE $\vec{L}\cdot\vec{J}$:

$$\vec{J} = \vec{L}+\vec{S} \Rightarrow \vec{S} = \vec{J}-\vec{L} \rightarrow \vec{S}^2 = (\vec{J}-\vec{L})^2 = \vec{J}^2 - 2\vec{J}\cdot\vec{L} + \vec{L}^2$$

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

$$\langle JM_J|\vec{J}\cdot\vec{L}|JM_J\rangle = \langle LSJM_J|\vec{J}\cdot\vec{L}|LSJM_J\rangle = \frac{1}{2}\langle \vec{J}^2 + \vec{L}^2 - \vec{S}^2\rangle$$

$$= \frac{1}{2}\hbar^2\left[J(J+1) + L(L+1) - S(S+1)\right]$$

$$\langle L_z\rangle = \frac{J(J+1)+L(L+1)-S(S+1)}{2J(J+1)}\hbar M_J$$

LIKEWISE, FOR $\langle S_z\rangle$, $S \leftrightarrow L$

$$\langle S_z\rangle = \frac{J(J+1)+S(S+1)-L(L+1)}{2J(J+1)}\hbar M_J$$

$$\Delta E = \frac{\mu_B B}{\hbar}\left(g_L \langle L_z \rangle + g_S \langle S_z \rangle\right) = \mu_B B\, g_J\, M_J$$

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

$\hookrightarrow$ "LANDÉ g FACTOR"

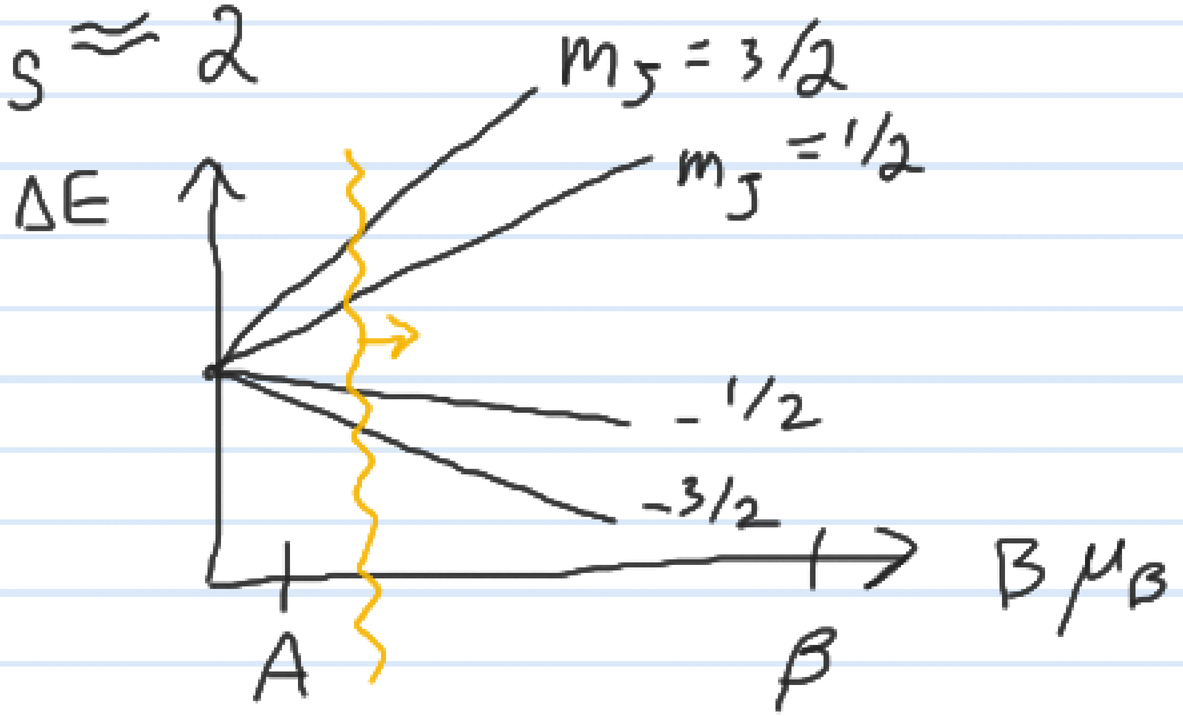
ELECTRON HAS EFFECTIVE SPIN OF J, MAG. MOMENT $\tilde{\mu}_J = \mu_B g_J \vec{J}/\hbar$

EX. Na $^2P_{3/2}$ EXCITED STATE. FIND ΔE vs. B, NEGLECT I

$L = 1$, $S = \frac{1}{2}$, $J = 3/2$; $g_L \approx 1$, $g_S \approx 2$

$g_J = 4/3$

$\Delta E = \frac{4}{3}\mu_B B M_J$; $M_J = \pm\frac{1}{2}, \pm\frac{3}{2}$



INCLUDE NUC. SPIN (I) FOOT 6.3.2

$$H_{HFS} = A\vec{I}\cdot\vec{J}/\hbar^2$$

$$H' = \frac{\mu_B B}{\hbar}\left(g_L L_z + g_S S_z + \underbrace{g_I I_z}_{}\right)$$

SMALL $\sim 10^{-4}$

USE PREVIOUS RESULT: $H' \approx H'' = \frac{\mu_B B}{\hbar}\left(g_J J_z + g_I I_z\right)$

FIRST CONSIDER HFS $\ll \mu_B B \ll$ FS

BASIS : $|M_I M_J\rangle$

$$\Delta E \cong \langle H''\rangle + \langle H_{HFS}\rangle = g_J \mu_B B M_J + \langle M_I M_J | A\vec{I}\cdot\vec{J}/\hbar^2 | M_I M_J\rangle$$

$$\langle M_I M_J | I_x J_x + I_y J_y + I_z J_z | M_I M_J\rangle = \langle M_I M_J | I_z J_z | M_I M_J\rangle$$

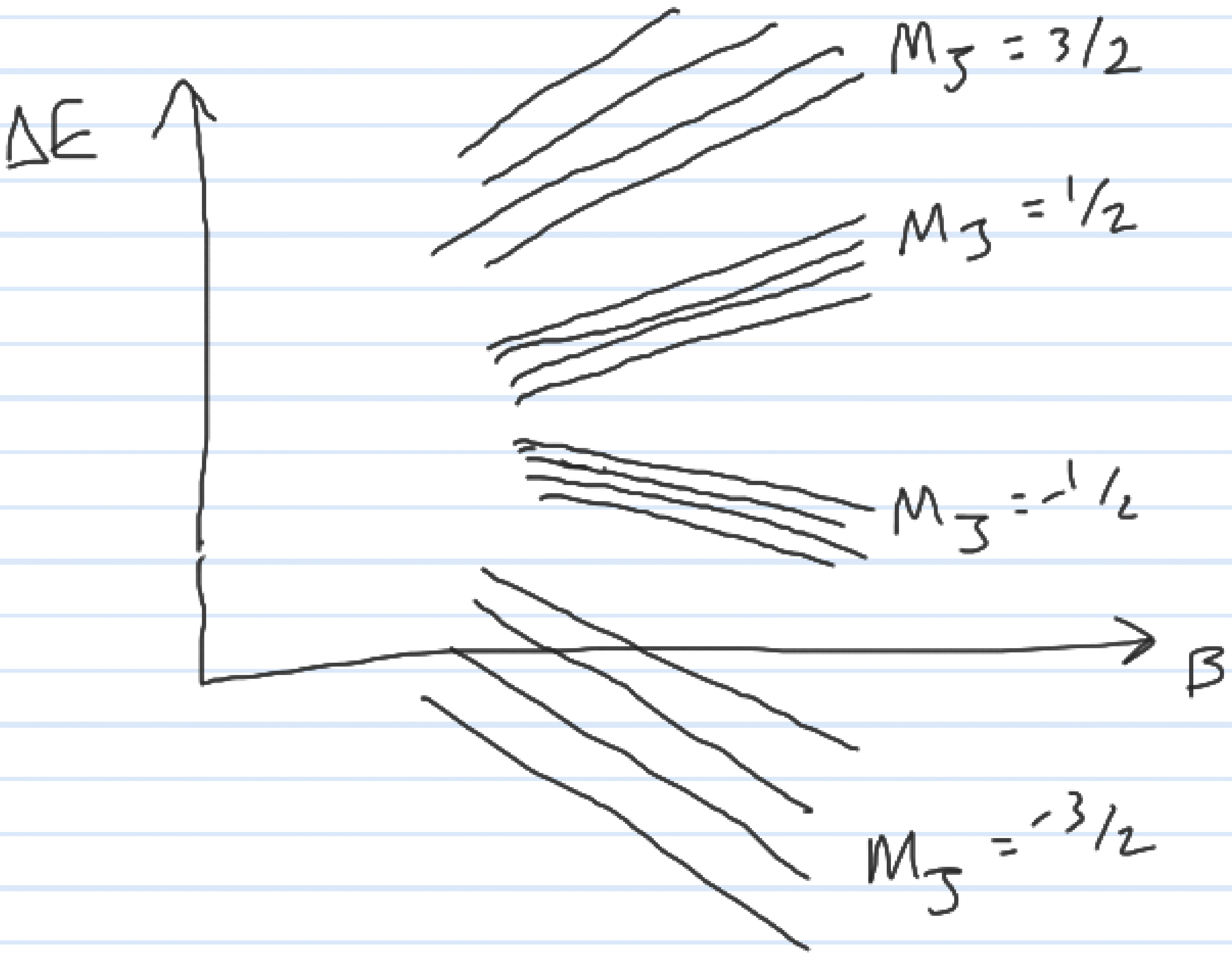
$$\langle M_I M_J | I_x J_x | M_I M_J\rangle = \underbrace{\langle M_I | I_x | M_I\rangle}_{0}\underbrace{\langle M_J | J_x | M_J\rangle}_{0} = 0$$

$$I_x = \frac{1}{2}(I_+ + I_-) \ ; \ \langle M_I | I_+ + I_- | M_I\rangle = 0$$

$$\langle M_I M_J | I_z J_z | M_I M_J\rangle = \langle M_I | I_z | M_I\rangle \langle M_J | J_z | M_J\rangle = \hbar^2 M_I M_J$$

$$\Delta E = g_J \mu_B B M_J + A M_I M_J$$

Ex. ^{23}Na, $I = \frac{3}{2}$, $M_I = \pm\frac{1}{2}, \pm\frac{3}{2}$



NEXT TIME: $\mu_B B \ll HFS \ll FS$ (EASY)

$\mu_B B \sim HFS \ll FS$ (MORE WORK BUT COOL)

3/30/2020 ATOMS IN MAGNETIC FIELDS

RECALL: FOR $\mu_B B \ll \beta$ (FINE STRUCTURE) $H_{FS} = \beta \vec{L}\cdot\vec{S}/\hbar^2$

$\vec{L}$ & $\vec{S}$ STRONGLY COUPLED → USE J EIGENSTATES

EFFECTIVE g FACTOR (LANDÉ) g_J

EFFECTIVE INTERACTION w/B FIELD: $H'_{eff} = g_J \mu_B \vec{B}\cdot\vec{J}/\hbar$

HYPERFINE STRUCTURE: $H_{HFS} = A\vec{I}\cdot\vec{J}/\hbar^2$

TOTAL HAMILTONIAN ($\vec{B} = B\hat{z}$)

$$H = A\vec{I}\cdot\vec{J}/\hbar^2 + \frac{\mu_B B}{\hbar}(g_J J_z + g_I I_z)$$

EIG. STATES $H|n\rangle = E_n|n\rangle$

TWO LIMITS:

1. STRONG FIELD LIMIT ($A \ll \mu_B B$)
   - 2ND TERM DOMINATES
   - APPROX. EIG. STATES $|M_J M_I\rangle$ $J_z|M_J M_I\rangle = \hbar M_J |M_J M_I\rangle$

$$E \approx \underbrace{\langle A\vec{I}\cdot\vec{J}/\hbar^2\rangle}_{A M_I M_J} + \mu_B B(g_J M_J + g_I M_I)$$

"PASCHEN-BACK REGIME"

EXAMPLE: ^{23}Na ($I = \frac{3}{2}$) $P_{1/2}$ EXCITED STATE (D1), STRONG-FIELD LIMIT

a) LABEL M_I, M_J FOR EACH

GIVEN: $g_J = 2/3$

$g_I \approx 0$

$A = h \times 94.4$ MHz

$E \approx A M_I M_J + g_J \mu_B B M_J$

b) FIND $E_2 - E_1$ FOR $\mu_B B \gg A$

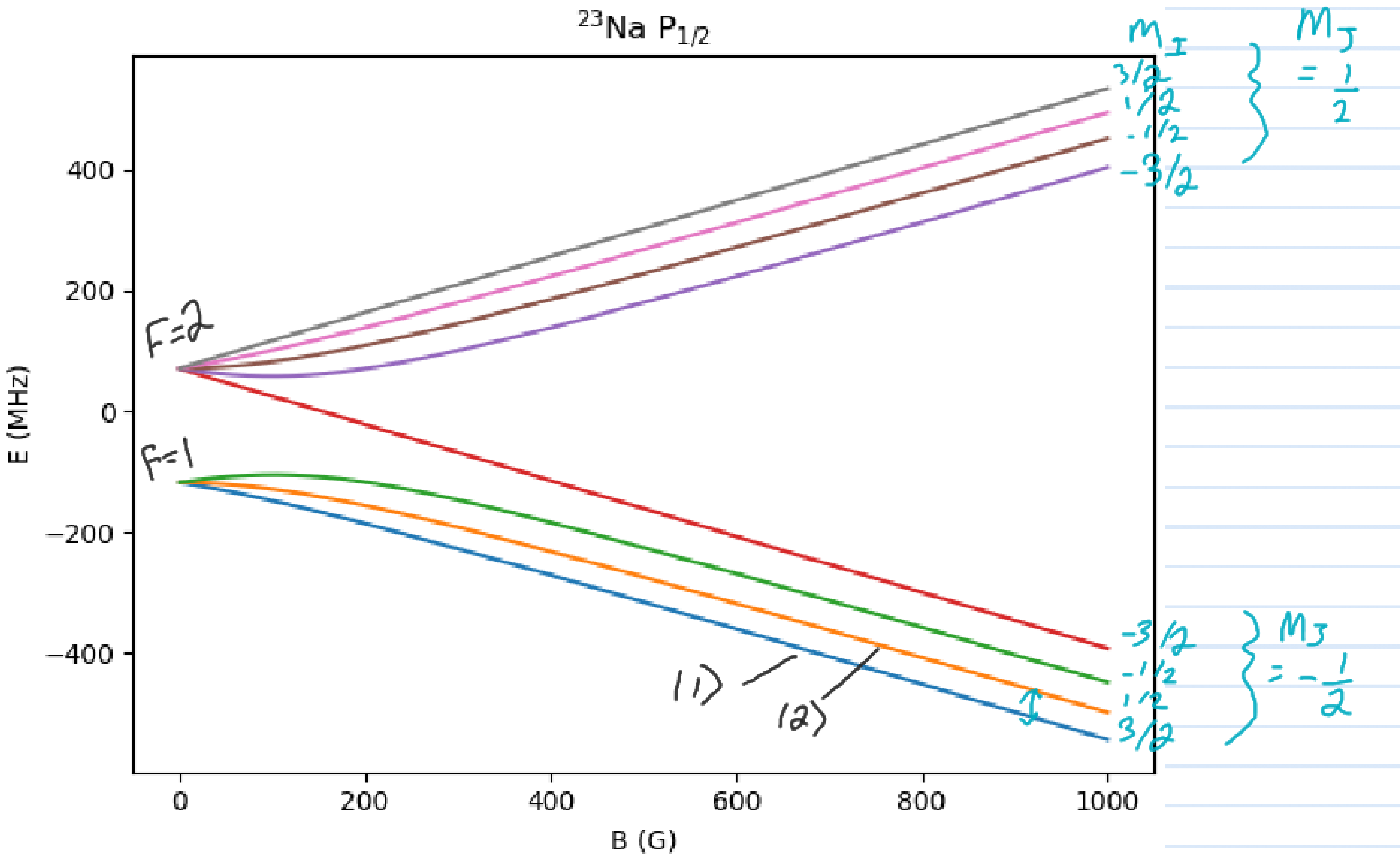
$|1\rangle \approx |M_J = -\frac{1}{2}, M_I = \frac{3}{2}\rangle$

$|2\rangle \approx |M_J = -\frac{1}{2}, M_I = \frac{1}{2}\rangle$

$E_2 - E_1 = A\left(\frac{1}{2}\right)\left(-\frac{1}{2}\right) - A\left(\frac{3}{2}\right)\left(-\frac{1}{2}\right)$

$= A\left(-\frac{1}{4} + \frac{3}{4}\right) = A/2$

$= \boxed{h \times 47.2 \text{ MHz}}$



WEAK-FIELD LIMIT ($\mu_B B \ll A$)

$$H = \underbrace{A\,\vec{I}\cdot\vec{J}/\hbar^2}_{\text{DOMINATES}} + \frac{\mu_B B}{\hbar}\left(g_J J_z + g_I I_z\right)$$

EIG. STATES: $|n\rangle \approx |F, M_F\rangle$, FIND EIG. VALS OF $\vec{I}\cdot\vec{J}$

$$\vec{F}^2 = (\vec{I}+\vec{J})^2 = \vec{I}^2 + 2\vec{I}\cdot\vec{J} + \vec{J}^2 \Rightarrow \vec{I}\cdot\vec{J} = \frac{1}{2}\left(\vec{F}^2 - \vec{I}^2 - \vec{J}^2\right)$$

NEXT: SHIFT DUE TO PERTURBATION $\propto B$

$$\Delta E = \langle F M_F | \frac{\mu_B B}{\hbar^2}\left(g_J J_z + g_I I_z\right) | F M_F \rangle$$

USE PROJECTION THEOREM

$$= g_F \mu_B B M_F$$

WHERE

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

"HYPERFINE g FACTOR"

EX. ^{23}Na $(I = 3/2)$ $P_{1/2}$ EXCITED STATE

a) ALLOWED $F = |I - J|, \ldots, I + J$

$= 1, 2$

b) GIVEN $g_I \approx 0$, $g_J = \frac{2}{3}$

$g_F(F{=}1) = -\frac{1}{6}$

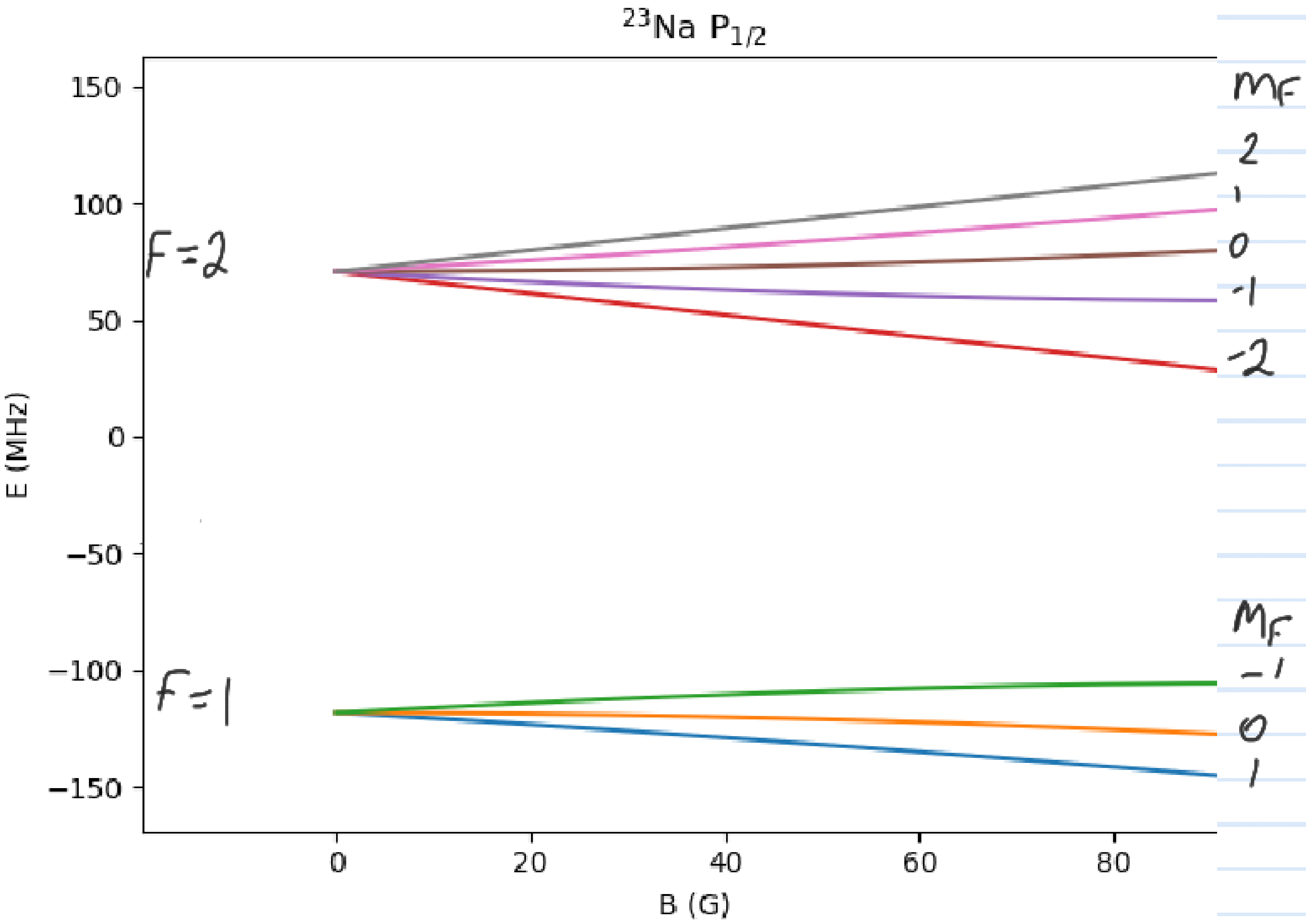
$g_F(F{=}2) = \frac{1}{6}$

LABEL F, M_F AT LOW FIELD

$F=2: \Delta E = g_F \mu_B B M_F$

$= \frac{1}{6} \mu_B B M_F$

$F=1: \Delta E = -\frac{1}{6} \mu_B B M_F$



EXACT SOLUTIONS : $H = A\,\tilde{I}\cdot\tilde{J}/\hbar^2 + \frac{\mu_B B}{\hbar}(g_J J_z + g_I I_z)$

- $[H, F_z] = 0$: FIND SIMULT. EIG. STATES
- IF $F_z|n\rangle = \hbar m_F |n\rangle$ THEN $|n\rangle$ IS A LINEAR COMBO OF STATES W/ F_z EIG. VAL $\hbar m_F$

SIMPLEST CASE: $I = \frac{1}{2}$, $J = \frac{1}{2}$ (i.e. GND STATE OF H)

STATES (BASIS) : $|m_I m_J\rangle$: $|\frac{1}{2}, \frac{1}{2}\rangle$, $|\frac{1}{2}, -\frac{1}{2}\rangle$, $|-\frac{1}{2}, \frac{1}{2}\rangle$, $|-\frac{1}{2}, -\frac{1}{2}\rangle$

F_z EIG. VALUES : 1 , 0 , 0 , -1

EXACT EIG. STATE!

COMBINE

EIG. STATE!

NEXT: FIND EXACT ENERGIES

4/1/2020 ATOMS IN B-FIELDS

HYPERFINE HAMILTONIAN: $H = A\vec{I}\cdot\vec{J}/\hbar^2 + \frac{\mu_B B}{\hbar}(g_I I_z + g_J J_z)$

EXACT SOLUTION

FIND SIMULT. EIG. STATES OF H AND $F_z = I_z + J_z$

SIMPLEST CASE: $I = \frac{1}{2}$, $J = \frac{1}{2}$ (ie HYDROGEN GND STATE)

ANALYZE IN $|m_I m_J\rangle$ BASIS

(REMINDER: LOW FIELD → $|F, m_F\rangle$ ARE ≈ EIG. STATES
HIGH FIELD → $|m_I m_J\rangle$ ARE ≈ EIG. STATES)

STATES: $|\frac{1}{2}, \frac{1}{2}\rangle$ $|\frac{1}{2}, -\frac{1}{2}\rangle$, $|-\frac{1}{2}, \frac{1}{2}\rangle$, $|-\frac{1}{2}, -\frac{1}{2}\rangle$

$m_F = m_I + m_J$: 1 $\underbrace{0 \quad 0}_{\text{FIND LINEAR COMBOS}}$ -1

EIG. STATE! FIND LINEAR COMBOS EIG. STATE!

ENERGY OF $|\frac{1}{2},\frac{1}{2}\rangle$: $\quad H|\frac{1}{2}\frac{1}{2}\rangle = E|\frac{1}{2}\frac{1}{2}\rangle$ $\quad \left[H = A\vec{I}\cdot\vec{J}/\hbar^2 + \frac{\mu_B B}{\hbar}(g_I I_z + g_J J_z) \right]$

$$\vec{I}\cdot\vec{J}|\tfrac{1}{2}\tfrac{1}{2}\rangle = \left[\tfrac{1}{2}(\cancelto{0}{I_+ J_-} + \cancelto{0}{I_- J_+}) + I_z J_z\right]|\tfrac{1}{2}\tfrac{1}{2}\rangle \quad \left[I_\pm = I_x \pm i I_y \;,\; J_\pm = J_x \pm i J_y\right]$$

$$= \tfrac{1}{4}\hbar^2|\tfrac{1}{2}\tfrac{1}{2}\rangle$$

$$H|\tfrac{1}{2}\tfrac{1}{2}\rangle = \tfrac{1}{4}A|\tfrac{1}{2}\tfrac{1}{2}\rangle + \mu_B B(g_I/2 + g_J/2)|\tfrac{1}{2}\tfrac{1}{2}\rangle$$

$$E_{\frac{1}{2}\frac{1}{2}} = \tfrac{1}{4}A + \tfrac{1}{2}\mu_B B(g_I + g_J)$$ "STRETCHED STATE"

ENERGY OF $|\text{-}\frac{1}{2}\,\text{-}\frac{1}{2}\rangle$: $\quad E_{-\frac{1}{2}-\frac{1}{2}} = \frac{1}{4}A - \frac{1}{2}\mu_B B(g_I + g_J)$

NOW: ENERGIES OF $M_F = 0$ STATES

NEED $|\psi\rangle = a|\frac{1}{2},\frac{-1}{2}\rangle + b|\frac{-1}{2},\frac{1}{2}\rangle$

SUCH THAT $\quad H|\psi\rangle = E|\psi\rangle$

SOLVE AS A MATRIX PROBLEM

$$H|\psi\rangle = E|\psi\rangle$$

$|\alpha\rangle = |\tfrac{1}{2}, -\tfrac{1}{2}\rangle$

$|\beta\rangle = |-\tfrac{1}{2}, \tfrac{1}{2}\rangle$

$$H\big(a|\alpha\rangle + b|\beta\rangle\big) = E\big(a|\alpha\rangle + b|\beta\rangle\big)$$

$\langle\alpha|\alpha\rangle = 1, \ \langle\alpha|\beta\rangle = 0$

$$\begin{cases} \langle\alpha|H|\alpha\rangle a + \langle\alpha|H|\beta\rangle b = E\,\langle\alpha|\big(a|\alpha\rangle + b|\beta\rangle\big) = Ea \\ \langle\beta|H|\alpha\rangle a + \langle\beta|H|\beta\rangle b = Eb \end{cases}$$

MATRIX EQUATION: $\begin{pmatrix} \langle\alpha|H|\alpha\rangle & \langle\alpha|H|\beta\rangle \\ \langle\beta|H|\alpha\rangle & \langle\beta|H|\beta\rangle \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = E\begin{pmatrix} a \\ b \end{pmatrix}$

NEED THE MATRIX ELEMENTS

$$H|\alpha\rangle = H|\tfrac{1}{2}, -\tfrac{1}{2}\rangle = \left[A\vec{I}\cdot\vec{J}/\hbar^2 + \frac{\mu_B}{\hbar}\left(g_I I_z + g_J J_z\right)\right]|\tfrac{1}{2}, -\tfrac{1}{2}\rangle$$

$$\vec{I}\cdot\vec{J}|\tfrac{1}{2}, -\tfrac{1}{2}\rangle = \left[\tfrac{1}{2}\big(\underbrace{I_+ J_-}_{\to 0} + I_- J_+\big) + I_z J_z\right]|\tfrac{1}{2}, -\tfrac{1}{2}\rangle$$

GENERAL RULE: $j_\pm|jm\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}\ |j, m\pm 1\rangle$

$$j_+|j=\tfrac{1}{2}, m=-\tfrac{1}{2}\rangle = \hbar\underbrace{\sqrt{\tfrac{1}{2}\left(\tfrac{1}{2}+1\right) - \left(-\tfrac{1}{2}\right)\left(-\tfrac{1}{2}+1\right)}}_{1}\,|j=\tfrac{1}{2}, m=\tfrac{1}{2}\rangle = \hbar\,|j=\tfrac{1}{2}, m=\tfrac{1}{2}\rangle$$

$$j_-|j=\tfrac{1}{2}, m=\tfrac{1}{2}\rangle = \hbar|j=\tfrac{1}{2}, m=-\tfrac{1}{2}\rangle$$

$$I_-J_+|\tfrac{1}{2},-\tfrac{1}{2}\rangle = \hbar^2|-\tfrac{1}{2},\tfrac{1}{2}\rangle$$

$$\vec{I}\cdot\vec{J}|\tfrac{1}{2},-\tfrac{1}{2}\rangle = \left[\tfrac{1}{2}I_-J_+ + I_zJ_z\right]|\tfrac{1}{2},-\tfrac{1}{2}\rangle = \tfrac{1}{2}\hbar^2|-\tfrac{1}{2},\tfrac{1}{2}\rangle - \tfrac{1}{4}\hbar^2|\tfrac{1}{2},-\tfrac{1}{2}\rangle = \hbar^2\left(\tfrac{1}{2}|\beta\rangle - \tfrac{1}{4}|\alpha\rangle\right)$$

$$H|\alpha\rangle = H|\tfrac{1}{2},-\tfrac{1}{2}\rangle = \left[A\vec{I}\cdot\vec{J}/\hbar^2 + \frac{\mu_B B}{\hbar}(g_I I_z + g_J J_z)\right]|\tfrac{1}{2},-\tfrac{1}{2}\rangle$$

$$j_z|jm\rangle = \hbar m|jm\rangle$$

$$= A\left(\tfrac{1}{2}|\beta\rangle - \tfrac{1}{4}|\alpha\rangle\right) + \mu_B B\left(g_I/2 - g_J/2\right)|\alpha\rangle$$

$$\langle\alpha|H|\alpha\rangle = -\tfrac{1}{4}A + \mu_B B(g_I - g_J)/2$$

$$\langle\beta|H|\alpha\rangle = \tfrac{1}{2}A$$

$$H|\beta\rangle = H|-\tfrac{1}{2},\tfrac{1}{2}\rangle = \left\{\frac{A}{\hbar^2}\left[\tfrac{1}{2}(I_+J_- + \cancel{I_-J_+}) + I_zJ_z\right] + \frac{\mu_B B}{\hbar}(g_I I_z + g_J J_z)\right\}|\overset{m_I}{-\tfrac{1}{2}},\overset{m_J}{\tfrac{1}{2}}\rangle$$

$$= A\tfrac{1}{2}|\tfrac{1}{2},-\tfrac{1}{2}\rangle - \tfrac{1}{4}A|-\tfrac{1}{2},\tfrac{1}{2}\rangle + \mu_B B\left(-\tfrac{1}{2}g_I + \tfrac{1}{2}g_J\right)|-\tfrac{1}{2},\tfrac{1}{2}\rangle$$

$$= \tfrac{1}{2}A|\alpha\rangle - \tfrac{1}{4}A|\beta\rangle - \mu_B B(g_I - g_J)/2\,|\beta\rangle$$

$$\langle\alpha|H|\beta\rangle = \tfrac{1}{2}A$$

$$\langle\beta|H|\beta\rangle = -\tfrac{1}{4}A - \tfrac{1}{2}\mu_B B(g_I - g_J)$$

MATRIX OF H ON $|\alpha\rangle, |\beta\rangle$ SUBSPACE

$$\underset{\uparrow \atop m_f=0}{[H]_0} = \begin{pmatrix} -\frac{1}{4}A + \frac{1}{2}\mu_B B(g_I - g_J) & \frac{1}{2}A \\ \frac{1}{2}A & -\frac{1}{4}A - \frac{1}{2}\mu_B B(g_I - g_J) \end{pmatrix} \equiv \begin{pmatrix} X & A/2 \\ A/2 & Y \end{pmatrix}$$

EIG. VALS: $$0 = \begin{vmatrix} X-E & A/2 \\ A/2 & Y-E \end{vmatrix} = (E-X)(E-Y) - (A/2)^2 = E^2 - (X+Y)E + (XY - A^2/4)$$

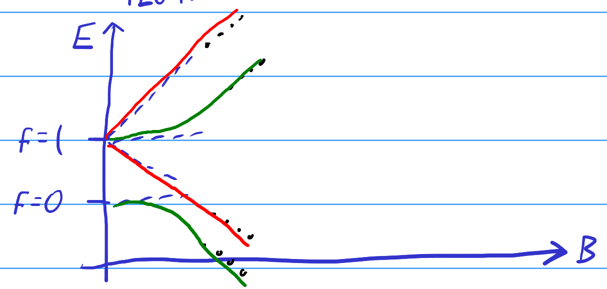
$$E = \left[X+Y \pm \sqrt{\underbrace{(X+Y)^2 - 4(XY - A^2/4)}_{X^2+2XY+Y^2-4XY+A^2 \;=\; (X-Y)^2 + A^2}} \right] / 2$$

$$= \left[X+Y \pm \sqrt{(X-Y)^2 + A^2} \right] / 2$$

$$X+Y = -\frac{1}{2}A \quad , \quad X-Y = \mu_B B(g_I - g_J)$$

$$E = -\frac{1}{4}A \pm \frac{1}{2}\sqrt{A^2 + (\mu_B B)^2 (g_I - g_J)^2}$$

PLOT:



$F = 0, 1$

g_F

MORE COMPLICATED CASE: $^{23}Na \left(I = \frac{3}{2}\right)$, GROUND STATE $J = \frac{1}{2}$ (OR $P_{1/2}$ EXC. STATE...)

$\lvert M_I M_J \rangle$ STATES	$M_F = M_I + M_J$	
$\frac{3}{2}\ \frac{1}{2}$	2	← EIG. STATE
$\frac{1}{2}\ \frac{1}{2}$	1	⇒ 2x2 MATRIX
$\frac{3}{2}\ -\frac{1}{2}$	1	
$\frac{1}{2}, -\frac{1}{2}$	0	⇒ 2x2
$-\frac{1}{2}, \frac{1}{2}$	0	
$\frac{3}{2}, -\frac{1}{2}$	-1	⇒ 2x2
$-\frac{1}{2}, -\frac{1}{2}$	-1	
$-\frac{3}{2}, -\frac{1}{2}$	-2	→ EIG. STATE

GENERAL RESULT: FOR $I = $ ANY, $J = \frac{1}{2}$

BREIT-RABI FORMULA:

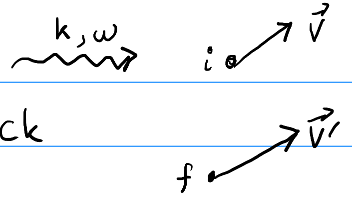
FOR NON-STRETCHED $E(m_F)_\pm = -\frac{1}{4}A + \mu_B B g_I m_F \pm \frac{A}{2}\sqrt{z^2 + 2m_F z + (I+\frac{1}{2})^2}$

WHERE $z = \mu_B B(g_J - g_I)/A$

FOR STRETCHED: $E_\pm = \frac{1}{2}AI \pm \mu_B B(g_I I + g_J/2)$

4/6/2020 Doppler Broadening

Doppler Shift:



$\omega = ck$

(INITIAL) $E_i = \hbar\omega_i$ $\quad |i\rangle = |1\rangle$

(FINAL) $E_f = \hbar\omega_f$ $\quad |f\rangle = |2\rangle$

MOMENTUM : $m\vec v + \hbar\vec k = m\vec v' \Rightarrow \vec v' = \vec v + \hbar k/m$

ENERGY : $\cancel{\tfrac{1}{2}mv^2} + \hbar\omega + \hbar\omega_i = \hbar\omega_f + \tfrac{1}{2}mv'^2$

$$= \hbar\omega_f + \tfrac{1}{2}m\left(\vec v + \hbar\vec k/m\right)^2$$

$$= \hbar\omega_f + \tfrac{1}{2}m\left(v^2 + \frac{2\hbar}{m}\vec k\cdot\vec v + \frac{\hbar^2k^2}{m^2}\right)$$

$$= \hbar\omega_f + \cancel{\tfrac{1}{2}mv^2} + \hbar\vec k\cdot\vec v + \frac{\hbar^2k^2}{2m}$$

SOLVE FOR ω:

$$\omega = \underbrace{(\omega_f - \omega_i)}_{\text{ATOMIC TRANSITION FREQ}} + \underbrace{\vec k\cdot\vec v}_{\text{DOPPLER SHIFT}} + \underbrace{\frac{\hbar k^2}{2m}}_{\text{RECOIL SHIFT}} \equiv \omega_0 + \vec k\cdot\vec v$$

DOPPLER SHIFT $\vec{k}\cdot\vec{v}$

IN ATOM FRAME: RED SHIFTED $\omega' < \omega$ FOR $k \cdot v > 0$

RESONANCE WHEN $\omega' = \omega_0$

$$\omega' = \omega - \vec{k}\cdot\vec{v} \Rightarrow \omega - \vec{k}\cdot\vec{v} = \omega_0$$

$$\Rightarrow \omega = \omega_0 + \vec{k}\cdot\vec{v} \quad \checkmark$$

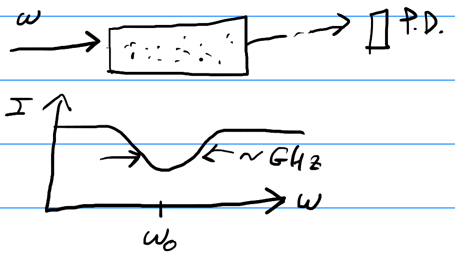
EXAMPLE: ^{23}Na, $T \sim 400K$; TYPICAL DOPPLER SHIFT

VELOCITY: $\frac{1}{2}mv^2 = \frac{3}{2}k_B T \Rightarrow v^2 = 3k_B T/m \Rightarrow V_{typ} = \sqrt{3k_B T/m}$; $m = 23$ amu

$V_{RMS} = 660$ m/s

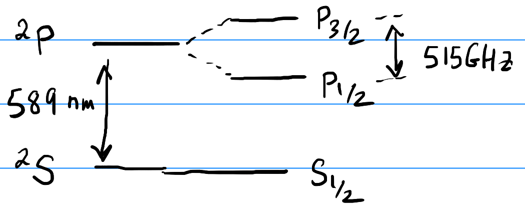
$k v_{rms} = \frac{2\pi}{\lambda} v_{rms}$; $\lambda = 589$ nm

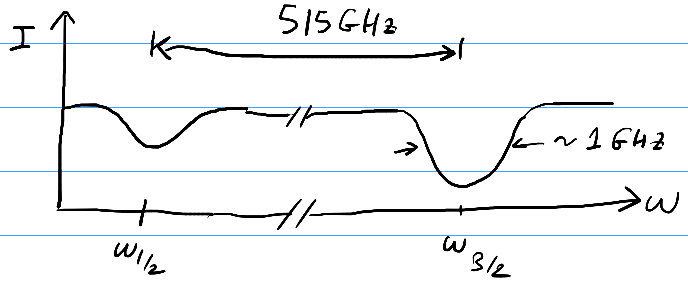
$= 2\pi \times \underline{1.1 \text{ GHz}}$



COMPARE to $\Gamma = 2\pi \times 9.8$ MHz $\ll k v_{rms}$

COMPARE TO FINE STRUCTURE OF ^{23}Na





CAN RESOLVE FINE STRUCTURE

BUT OFTEN NOT HYPERFINE STRUCTURE, $\Delta\nu_{HFS} \sim 1\,MHz$ to $\sim 10\,GHz$

USEFUL TO BE ABLE TO AVOID DOPPLER BROADENING

→ SATURATED ABSORPTION SPECTROSCOPY

DOPPLER BROADENING LINESHAPE

ABSORPTION

$$\frac{dI}{dz} = -a(\omega)\, I$$

$$a(\omega) = \frac{a_0}{1 + S + \left[\frac{2}{\Gamma}(\omega - \omega_0)\right]^2} \quad ; \quad a_0 = \frac{6\pi}{k_0^2} n_a \quad ; \quad k_0 = \omega_0 / c$$

$\uparrow$ ATOMIC DENSITY

IF ATOMS ALL HAVE VELOCITY $\vec{v}$: $a(\omega, \vec{v}) = a(\omega - \vec{k}\cdot\vec{v})$

DEFINE ABSORPTION CROSS-SECTION: $\sigma(\omega) = \dfrac{\sigma_0}{1 + \left[\frac{2}{\Gamma}(\omega - \omega_0)\right]^2}$; $\sigma_0 = \dfrac{6\pi}{k_0^2}$

$$= \left[a(\omega)/n_a\right]\Big|_{S=0}$$

- INTERPRET: σ = CROSS-SECTIONAL AREA OF GND STATE ATOM (AS SEEN BY PHOTON)

VELOCITY DISTRIBUTION: $\tilde{n}(v_z)$

- CONSIDER $\vec{k} = k\hat{z} \Rightarrow \vec{k}\cdot\vec{v} = k v_z$

$dn_a = \tilde{n}(v_z)\, dv_z$ = DENSITY OF ATOMS W/VELOCITY v_z IN dv_z

$$da = \frac{\sigma_0\, dn_a}{1 + s + \left[\frac{2}{\Gamma}(\omega - \omega_0 - k v_z)\right]^2}$$

CALCULATE ABSORPTION OF WEAK PROBE BEAM ($s \ll 1$) i.e. $I \ll I_{SAT}$

$$a(\omega) = \int da = \int_{-\infty}^{\infty} \tilde{n}(v_z) \frac{\sigma_0}{1 + \left[\frac{2}{\Gamma}(\omega - \omega_0 - k v_z)\right]^2}\, dv_z = \int_{-\infty}^{\infty} \tilde{n}(v_z)\, \sigma(\omega - k v_z)\, dv_z$$

LET'S EVALUATE FOR HIGH TEMPERATURES ($k v_{rms} \gg \Gamma$)

MAXWELL-BOLTZMANN DISTRIBUTION: $\tilde{n}(v_z) \propto e^{-\beta \frac{1}{2} m v_z^2}$; $\beta = \frac{1}{k_B T}$

NORMALIZE: $\int_{-\infty}^{\infty} \tilde{n}(v_z)\, dv_z = n_a$

$$\tilde{n}(v_z) = \frac{n_a}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2} v_z^2/\sigma^2} \Rightarrow \frac{1}{\sigma^2} = \beta m \Rightarrow \sigma = \frac{1}{\sqrt{\beta m}} = \sqrt{\frac{k_B T}{m}}$$

$$= n_a \sqrt{\frac{m}{2\pi k_B T}}\, e^{-\frac{1}{2} v_z^2 \frac{m}{k_B T}}$$

// DEFINE $u = \sqrt{2 k_B T / m}$

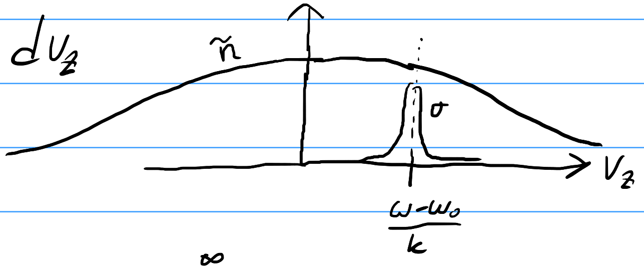
$$= \frac{n_a}{u\sqrt{\pi}} e^{-v_z^2/u^2}$$

NORMALIZED LORENTZIAN: $L(x) = \frac{1}{\pi} \frac{\Gamma/2}{x^2 + (\Gamma/2)^2}$

$$\Rightarrow \int_{-\infty}^{\infty} L(x)\,dx = 1$$

CROSS-SECTION: $\sigma(\omega) = \frac{\sigma_0}{1 + \left[\frac{2}{\Gamma}(\omega-\omega_0)\right]^2} = \frac{\sigma_0 (\Gamma/2)^2}{(\Gamma/2)^2 + (\omega-\omega_0)^2} = \frac{\pi \sigma_0 \Gamma}{2} L(\omega-\omega_0)$

$$a(\omega) = \int_{-\infty}^{\infty} \tilde{n}(v_z)\, \sigma(\omega - k v_z)\, dv_z$$



$\omega - \omega_0 = k v_z$

HIGH-T REGIME

LOR. WIDTH: $\Delta v_z = \Gamma/k \ll v_{RMS} \sim u$

$\Rightarrow \Delta v_z\,(\text{LOR.}) \ll u$

$(x = k v_z)$

$$\approx \tilde{n}\left(\frac{\omega-\omega_0}{k}\right) \int_{-\infty}^{\infty} \sigma(\omega - k v_z)\, dv_z = \tilde{n} \int_{-\infty}^{\infty} \frac{\pi \sigma_0 \Gamma}{2} L(\omega - k v_z - \omega_0)\, dv_z = \frac{\tilde{n}(\cdot)\, \pi \sigma_0 \Gamma}{2} \int_{-\infty}^{\infty} L(x) \frac{dx}{k}$$

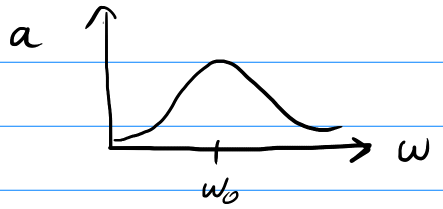
TAKE THE INTEGRAL:

$$a(\omega) \approx \frac{\pi \sigma_0 \Gamma}{2k} \tilde{n}\left(v_z = \frac{\omega-\omega_0}{k}\right) = \frac{\sigma_0 \Gamma \sqrt{\pi}}{2ku} n_a \, e^{-(\omega-\omega_0)^2/(ku)^2}$$

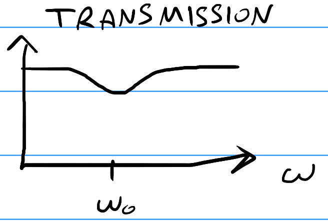
CENTER: $\omega = \omega_0$; $1/e$ WIDTH: ku

HALF WIDTH: $\frac{1}{2} = e^{-(\delta_{1/2})^2/(ku)^2} \rightarrow \ln(2) = (\delta_{1/2})^2/(ku)^2 \rightarrow \delta_{\frac{1}{2}} = ku\sqrt{\ln 2}$

FWHM $\Delta\omega_D = 2\delta_{\frac{1}{2}} = 2\sqrt{\ln 2}\, ku$



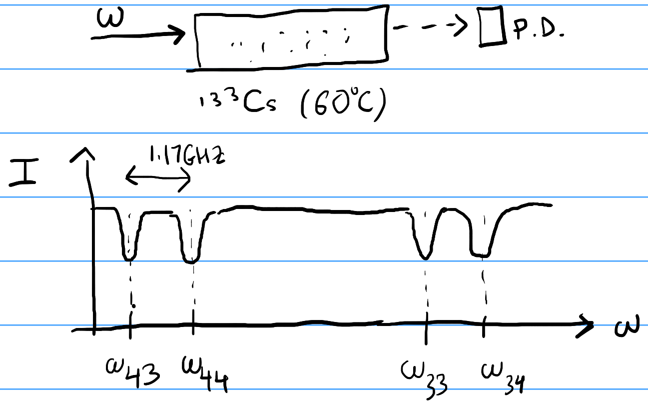
$\Rightarrow$



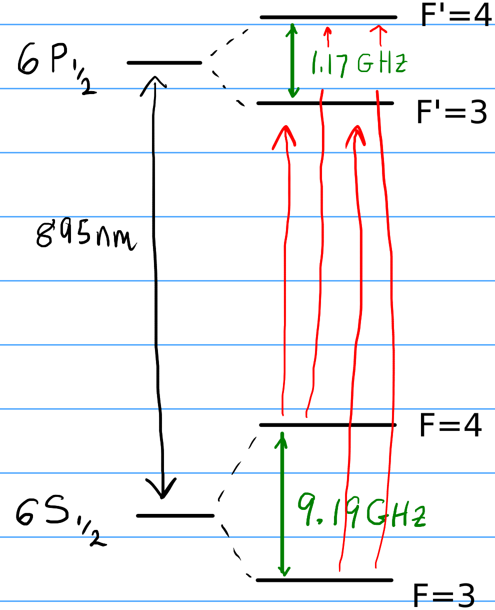
4/8/2020 SATURATED ABSORPTION SPECTROSCOPY

WARM-UP: DOPPLER BROADENING

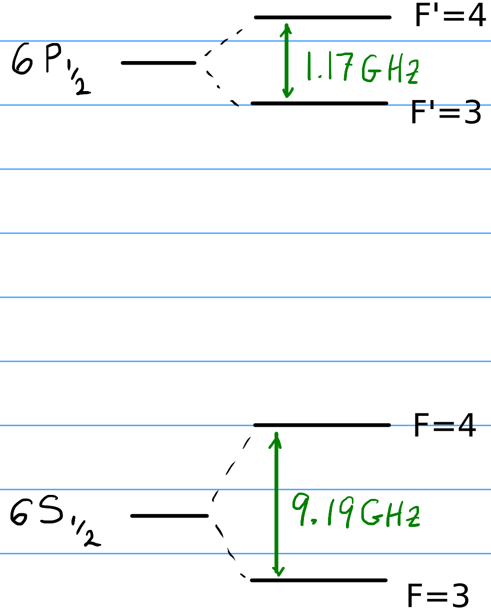
1) $T = 60^\circ C$, FIND FWHM (DOPPLER) $\Delta\omega_D = 2\pi \times 0.38\,GHz$
2) COMPARE $\Delta\omega_D$ TO HFS: IS HFS RESOLVED?
3) Sketch Transmission vs. ω



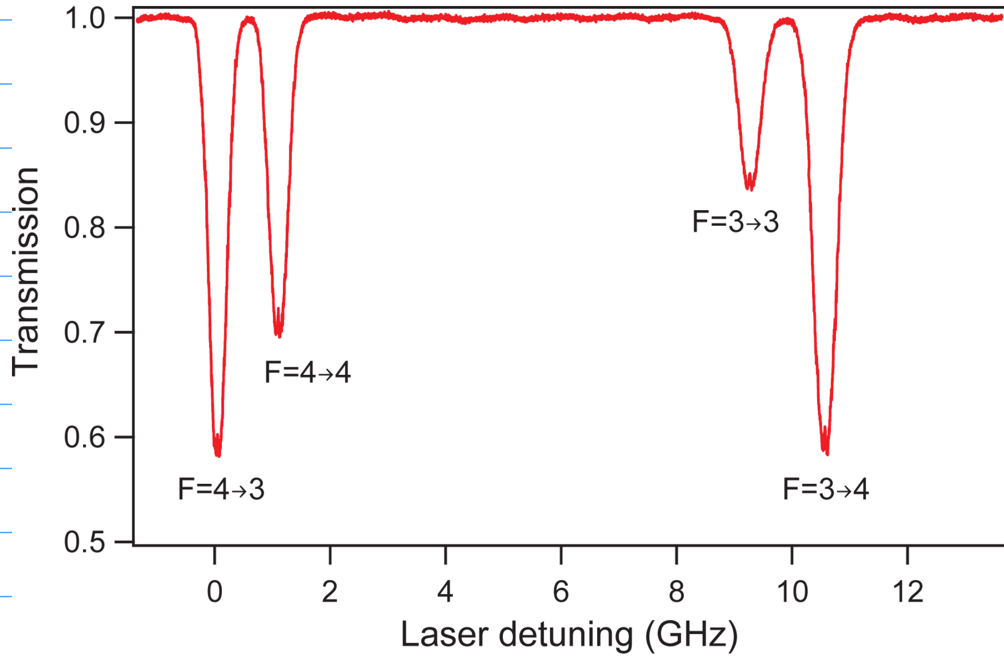
^{133}Cs D1 Line



^{133}Cs D1 Line



Doppler-broadened absorption, Cs D1 line



Gruet et al, Opt. Express 21, 5781-5792 (2013)

SATURATED ABSORPTION

RECALL: ABSORPTION CROSS-SECTION

$$\sigma(\omega) = \frac{\sigma_0}{1 + \left[\frac{2}{\Gamma}(\omega - \omega_0)\right]^2}$$

INCLUDE SATURATION $S = I/I_{SAT}$

SATURATED SCATTERING CROSS-SECTION (SOME PROBABILITY TO BE IN EXCITED STATE)

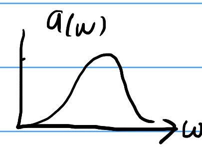
$$\sigma_S(\omega) = \frac{\sigma_0}{1 + S + \left[\frac{2}{\Gamma}(\omega - \omega_0)\right]^2}$$

STEADY STATE: $\rho_{11} - \rho_{22} = \dfrac{1 + (2\delta/\Gamma)^2}{1 + S + (2\delta/\Gamma)^2}$, $\delta = \omega - \omega_0$

$$\Rightarrow \sigma_S(\omega) = (\rho_{11} - \rho_{22})\,\sigma(\omega)$$

PREVIOUSLY, FOUND ABSORPTION COEF.:

$$a(\omega) = \int_{-\infty}^{\infty} \tilde{n}(v_z)\,\sigma(\omega - k v_z)\,dv_z \quad , \text{ FOR } S \ll 1 \rightarrow \text{GAUSSIAN}$$



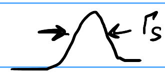
INCLUDE SATURATION:

$$a(\omega) = \int_{-\infty}^{\infty} \tilde{n}(v_z)\,\sigma_S(\omega - k v_z)\,dv_z = \int_{-\infty}^{\infty} (\rho_{11} - \rho_{22})\,\tilde{n}(v_z)\,\sigma(\omega - k v_z)\,dv_z$$

$$= \int_{-\infty}^{\infty} \left[\tilde{n}_1(v_z) - \tilde{n}_2(v_z) \right] \sigma(\omega - k v_z)\,dv_z$$

$$\tilde{n}_1(v_z) = \rho_{11}(\omega - k v_z)\,\tilde{n}(v_z) \quad ; \quad \rho_{11} = 1 - \rho_{22}$$

$$\rho_{22}(\omega) = \frac{1}{2} \frac{S}{1 + S + \left[\frac{2}{\Gamma}(\omega - \omega_0)\right]^2}$$



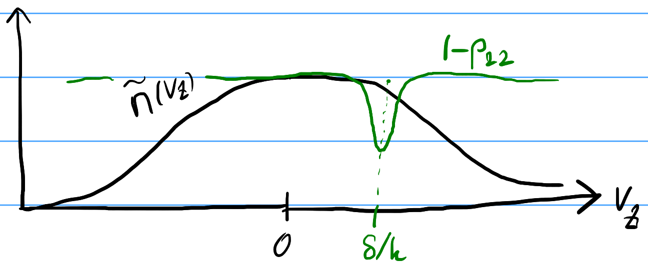
$$= \frac{1}{2} \frac{S}{1+S} \frac{1}{1 + \left[\frac{2}{\Gamma_S}(\omega - \omega_0)\right]^2} \quad ; \text{ WHERE } \Gamma_S = \Gamma\sqrt{1+S} \quad \text{"POWER BROADENING"}$$

GROUND STATE DISTRIBUTION

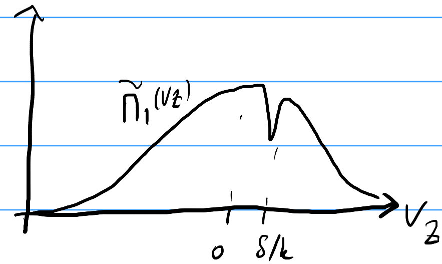
$$\tilde{n}_1(v_z) = \tilde{n}(v_z)\left[1-\rho_{22}(\omega - k v_z)\right]$$

PEAK WHEN $\omega - k v_z = \omega_0$

$k v_z = \omega - \omega_0 = \delta$

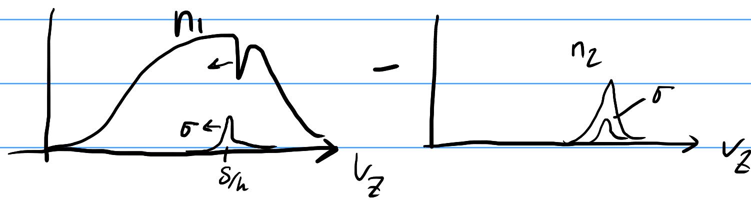


MULTIPLY:

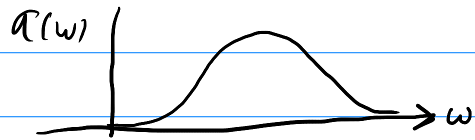


"BENNETT HOLE"

REDUCES ABSORPTION:



STILL GAUSSIAN:

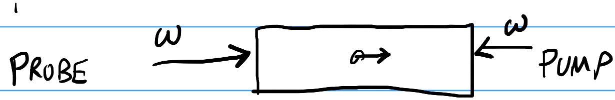


(BUT SMALLER THAN AT $s \ll 1$)

IS THERE A WAY TO "SEE" THE BENNETT HOLE?

YES! USE TWO LASER BEAMS

FOR EXAMPLE:



PUMP (LARGE S), PROBE ($S \ll 1$)

↳ BURNS A HOLE IN $\tilde{n}_1(v_z)$ AT $\omega = \omega_0 - kv_z$ $\left(\omega + kv_z = \omega_0 \right)$

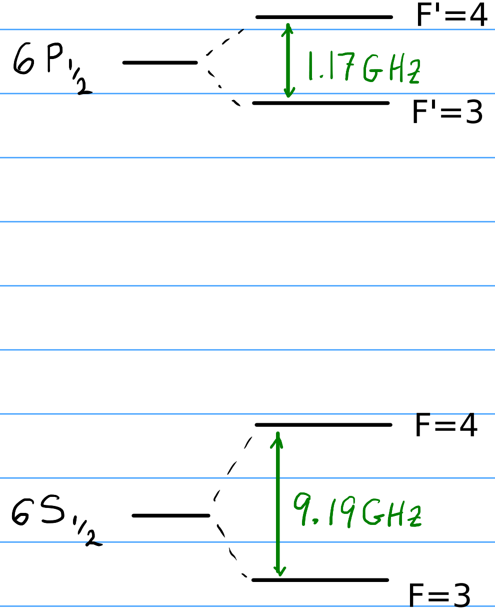
$kv_z = \omega_0 - \omega$

PROBE RESONANT WITH ATOMS WHERE $\omega = \omega_0 + kv_z' \Rightarrow kv_z' = \omega - \omega_0$

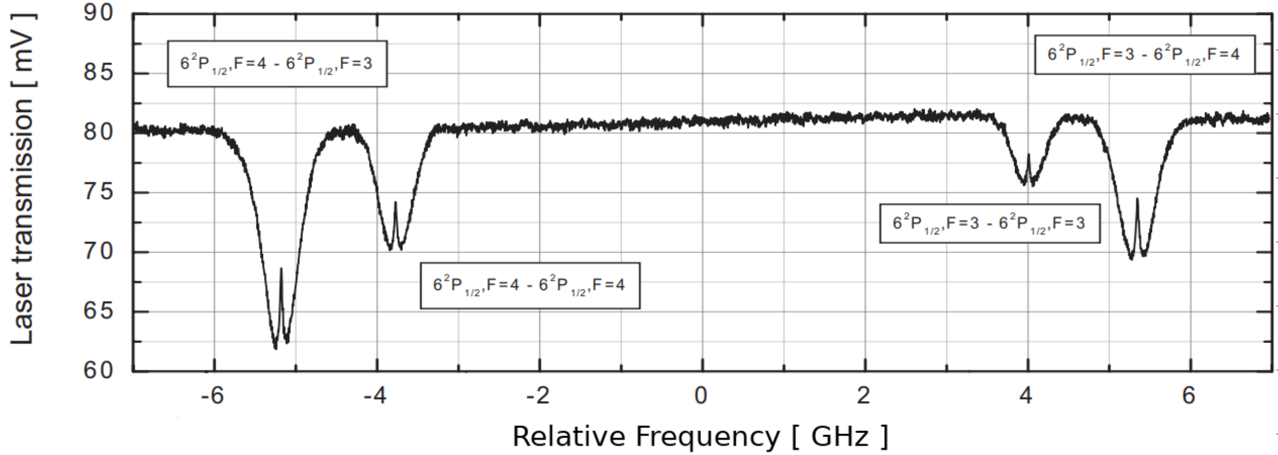
PUMP ONLY REDUCES ABSORPTION WHEN $v_z = v_z' \Rightarrow \omega_0 - \omega = \omega - \omega_0$

$2\omega_0 = 2\omega \Rightarrow \boxed{\omega = \omega_0}$

^{133}Cs D1 Line

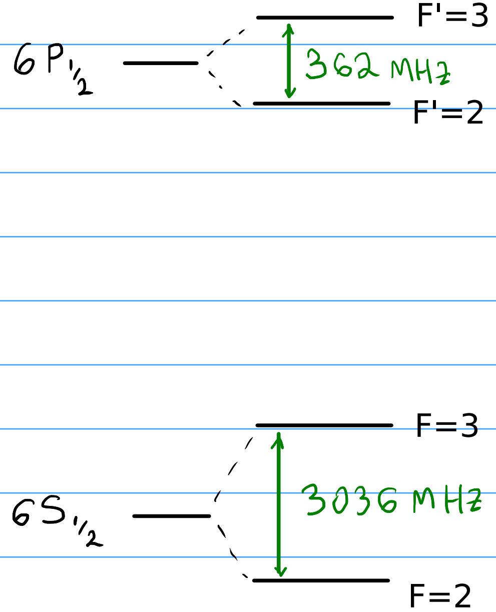


Sub-Doppler Features (Cs D1 line)

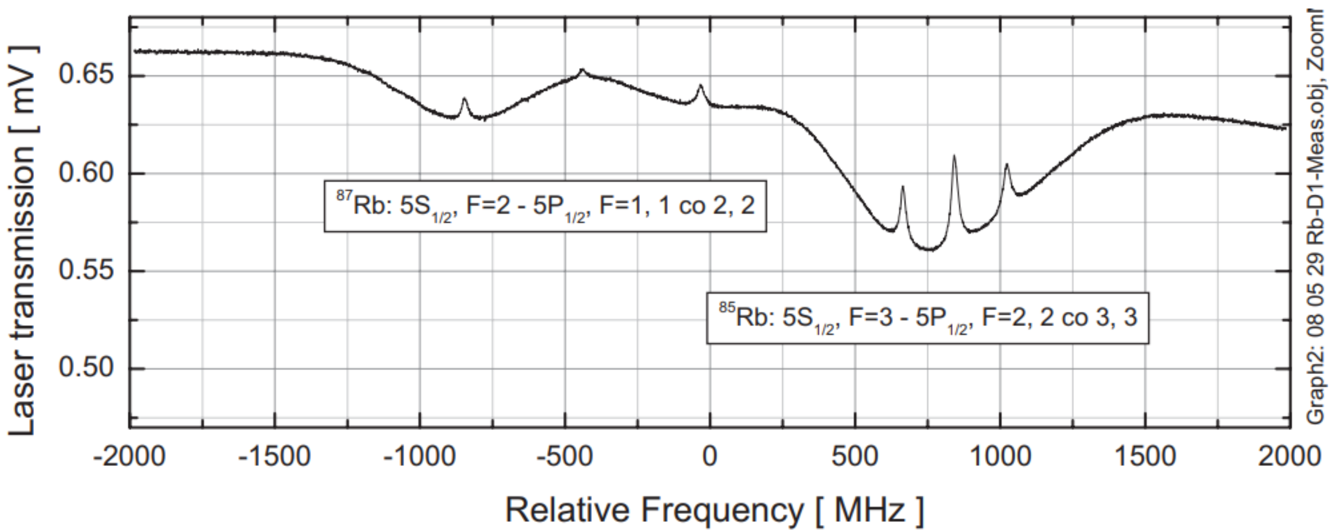


sacher-laser.com "Cesium D1"

^{85}Rb D1 Line

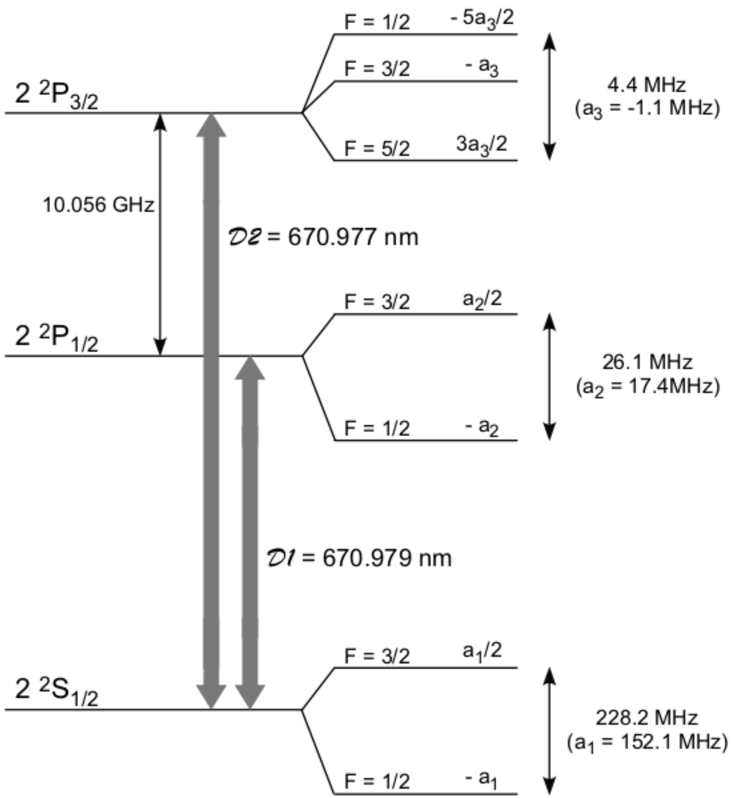


Excited-state crossover features (Rb D1 line)



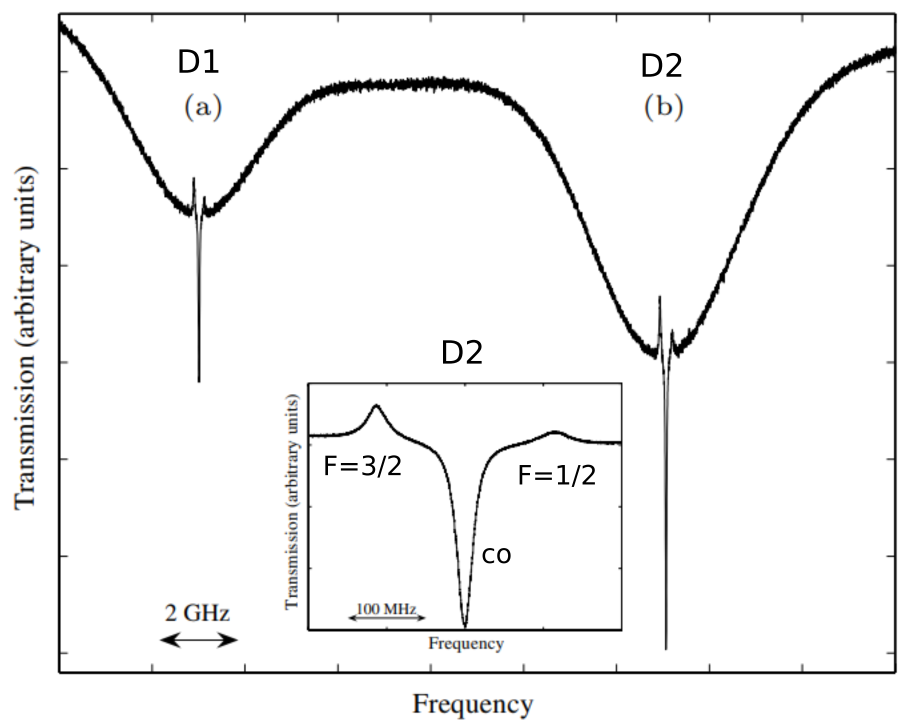
sacher-laser.com "Rubidium D1"

^{6}Li D1 & D2 Lines ($\Gamma = 5.8$ MHz)



M. Gehm, "Properties of 6Li"

Ground-state crossover features (Li-6)



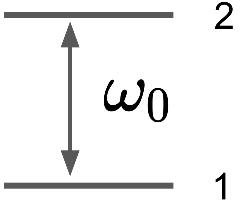
Fuchs et al, J. Phys. B: At. Mol. Opt. Phys. 39, 3479 (2006)

PHY 446 Lecture 22

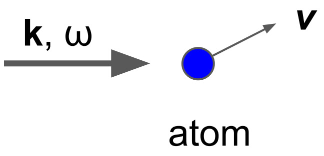
Crossover resonances in saturated absorption spectroscopy

Ariel Sommer
April 13, 2020
Lehigh University

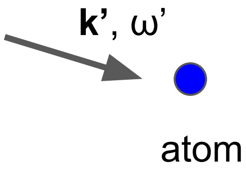
Doppler Shift (Non-Relativistic)



Lab frame:



In atom's rest frame:



Doppler effect (*v* << *c*): $\omega' \approx \omega\,(1 - v_z/c) = \omega - k v_z$

Resonance condition
(analyzed in atom's frame):

$$\omega' = \omega_0 + \cancel{\frac{\hbar k'^2}{2m}}$$

Recoil shift (small)

In lab frame:

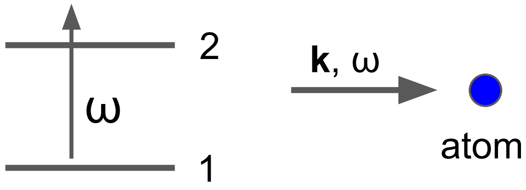
$$\omega - k v_z = \omega_0$$

$$\omega = \omega_0 + k v_z$$

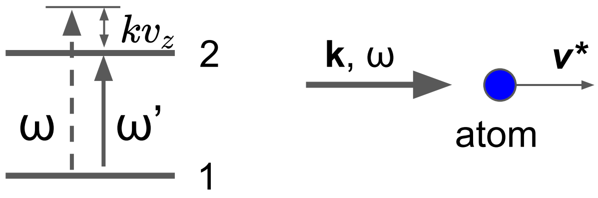
Doppler broadening

Consider light at $\omega > \omega_0$

$v_z = 0$: Not resonant



$kv_z = \omega - \omega_0$: Resonant



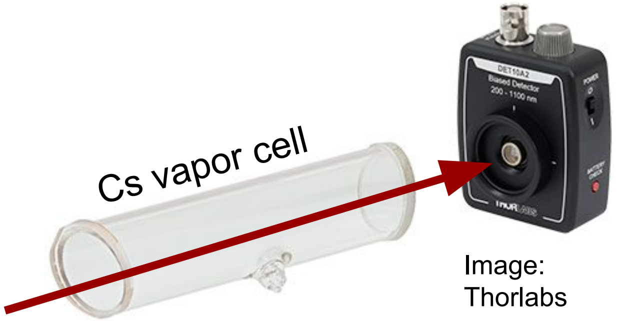
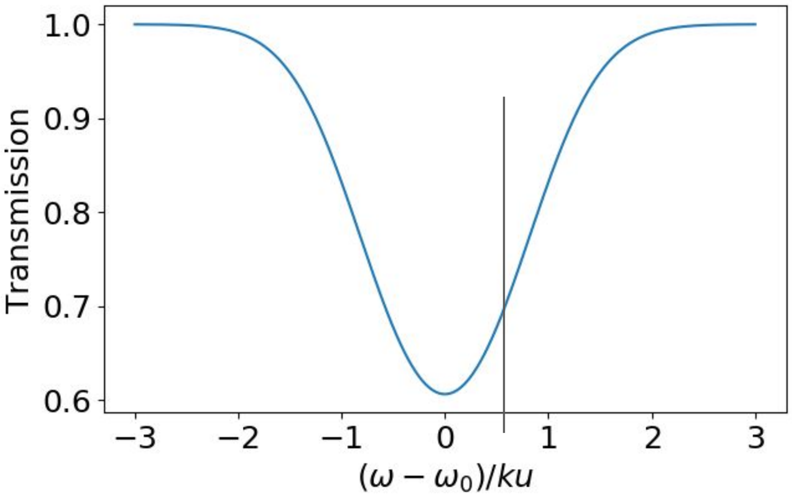


Image: Thorlabs



Doppler broadening

Velocity distribution $$\tilde{n}(v_z) = \frac{n_a}{u\sqrt{\pi}} e^{-v_z^2/u^2}$$

Typical speed $$u = \sqrt{2k_B T/m}$$

Doppler-broadened absorption coefficient:

$$a(\omega) = \frac{\sigma_0 \Gamma \sqrt{\pi} n_a}{2ku} e^{-(\omega-\omega_0)^2/(ku)^2}$$

FWHM: $$\Delta\omega_D = 2\sqrt{\ln 2}\, ku \approx 1.7ku$$

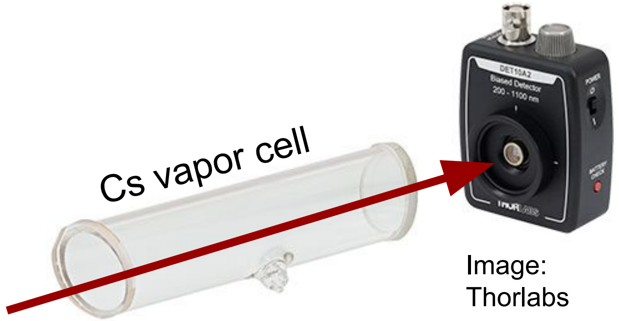
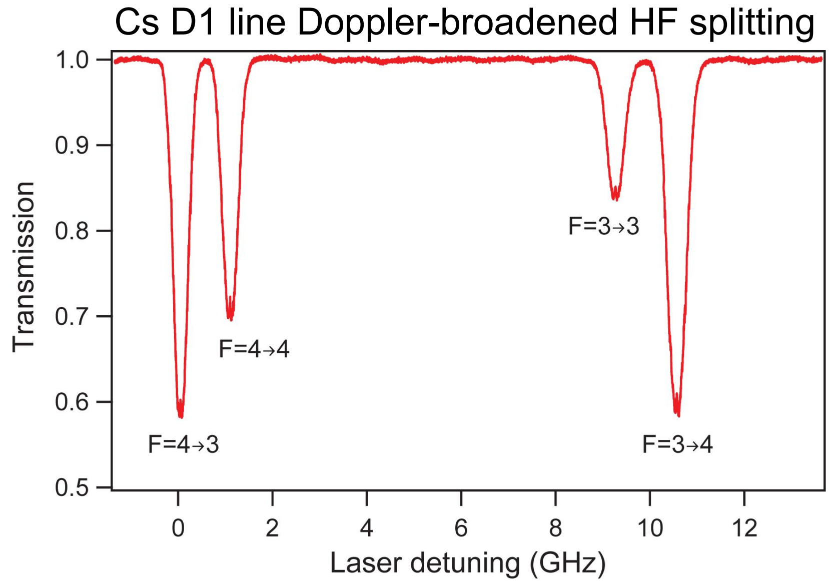
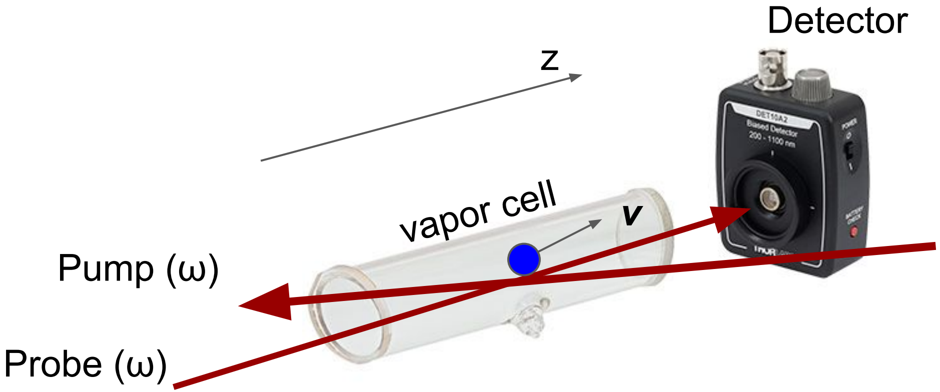


Image: Thorlabs

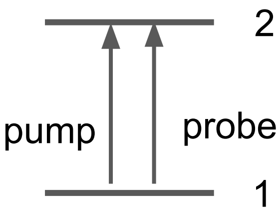


Gruet et al, Opt. Express 21, 5781-5792 (2013)

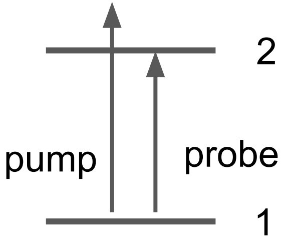
Saturated Absorption Spectroscopy



$$\omega = \omega_0, v_z = 0:$$



$$\omega > \omega_0,$$
$$kv_z = \omega - \omega_0$$

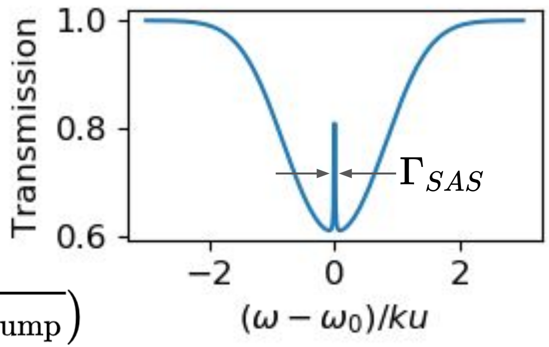


(atom’s frame)

Probe resonance: $\omega - kv_z = \omega_0$

Pump resonance: $\omega + kv_z = \omega_0$

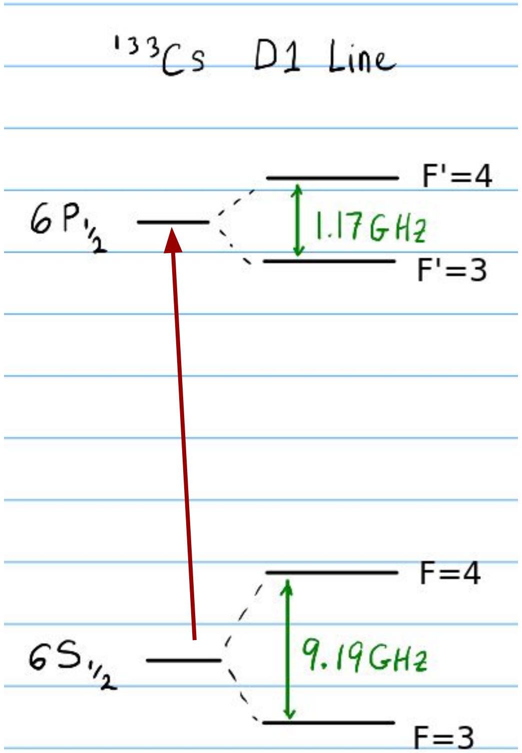
$\omega=\omega_0$: pump and probe both resonant when $v_z=0$



Narrow peak at $\omega=\omega_0$; FWHM $\Gamma_{SAS} = \frac{1}{2}\Gamma\left(1+\sqrt{1+s_{\text{pump}}}\right)$

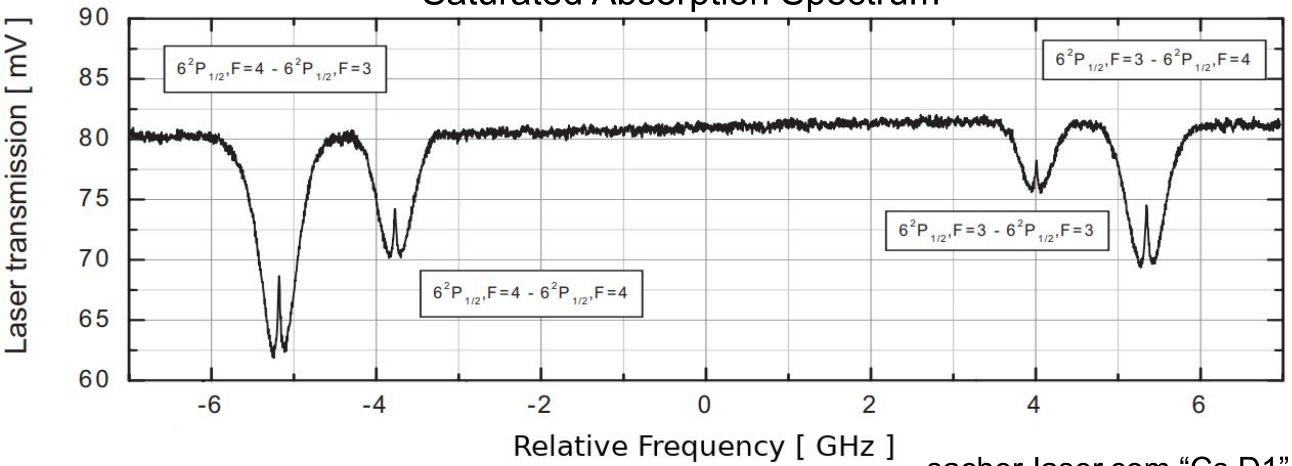
SAS Example: ^{133}Cs D1 line

All hyperfine transitions Doppler-resolved –> 2-level system within each Doppler profile



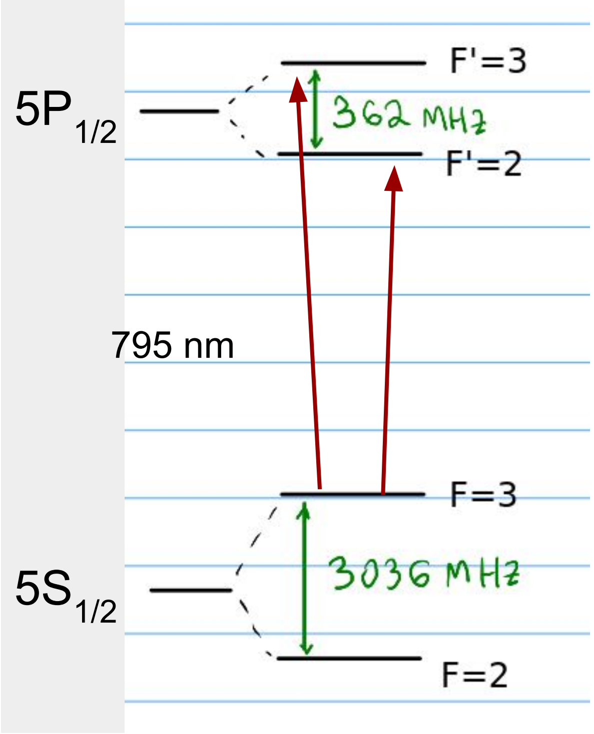
Doppler width: $\Delta\omega_D \approx 2\pi \times 0.38\,\mathrm{GHz}$ (assuming T=60 C)

Saturated Absorption Spectrum



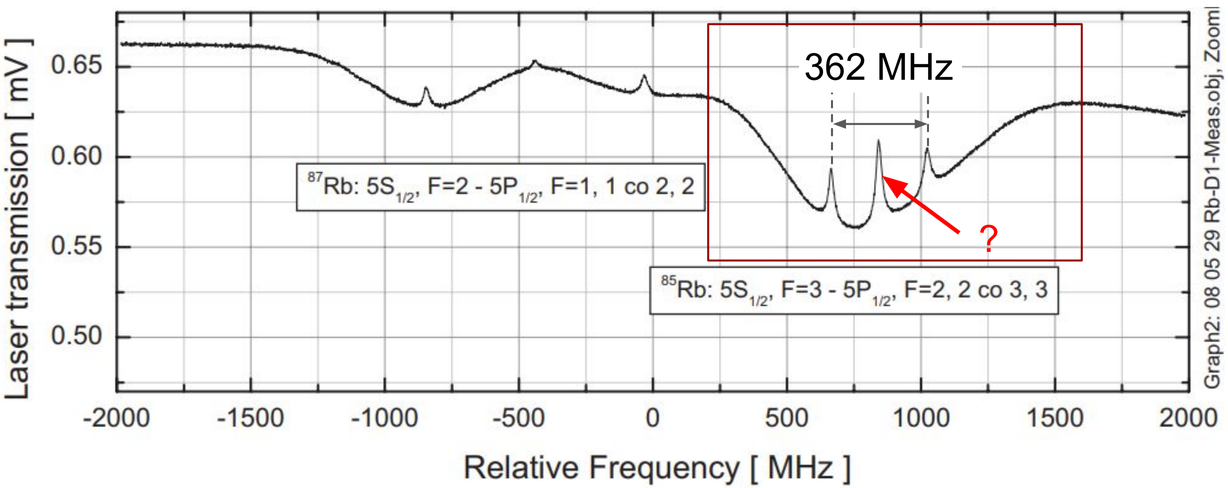
sacher-laser.com “Cs D1”

SAS Example 2: ^{85}Rb D1 line



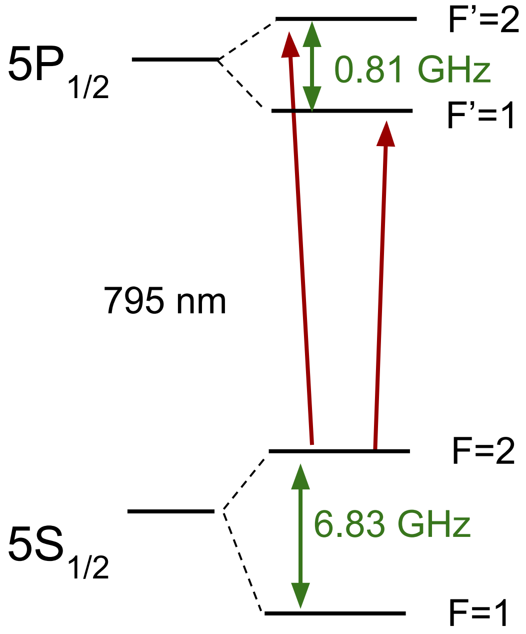
Doppler width: $\Delta\omega_D \approx 2\pi \times 0.53\,\mathrm{GHz}$ (assuming T=60 C)

Excited states not Doppler-resolved



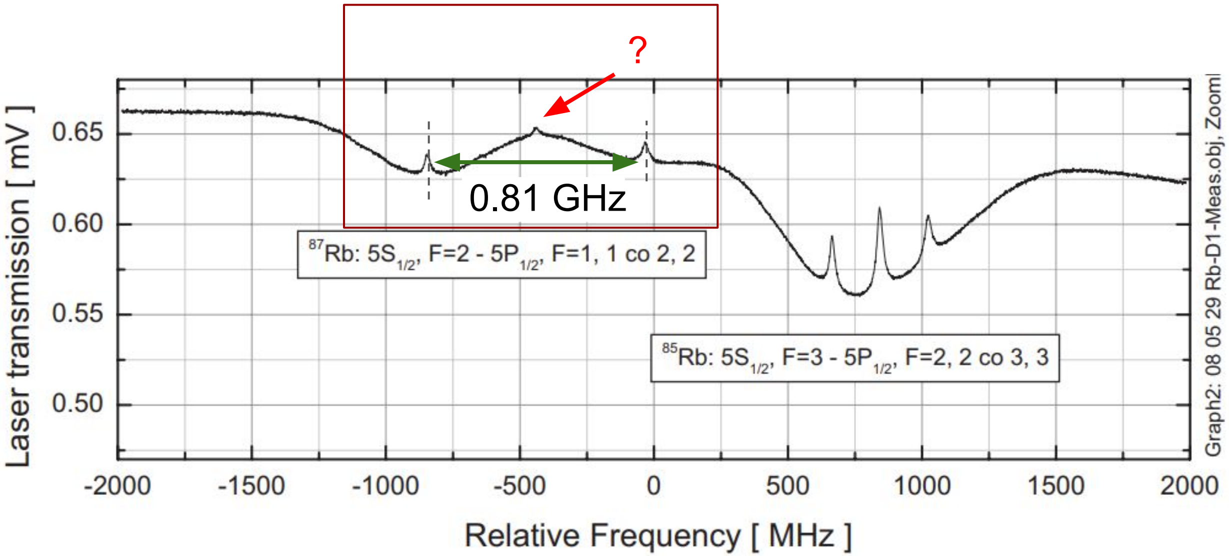
sacher-laser.com “Rb D1”

SAS Example 3: ^{87}Rb D1 line



Doppler width: $\Delta\omega_D \approx 2\pi \times 0.53\,\mathrm{GHz}$ (assuming T=60 C)

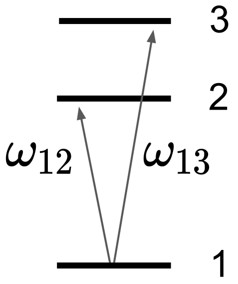
Excited states *just barely* Doppler-resolved



sacher-laser.com "Rb D1"

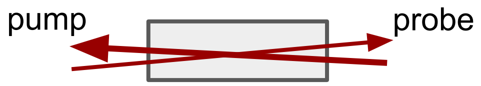
SAS Crossover Resonances (Excited State)

3-level “V”



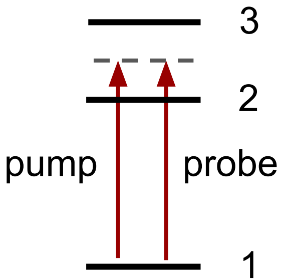
Counter-propagating beams with

$$\omega = (\omega_{12} + \omega_{13})/2$$

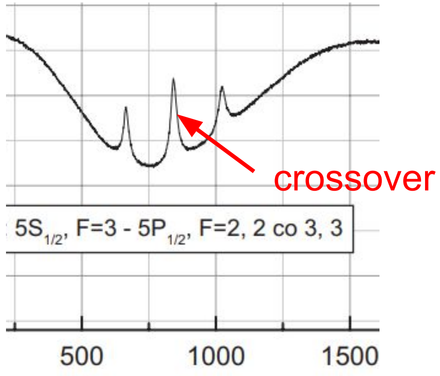


Atoms Doppler-shifted into resonance:

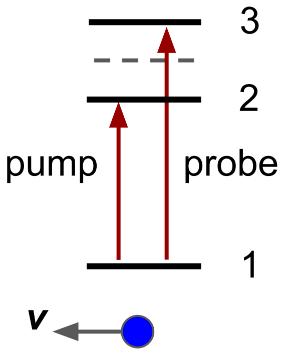
$v_z = 0:$



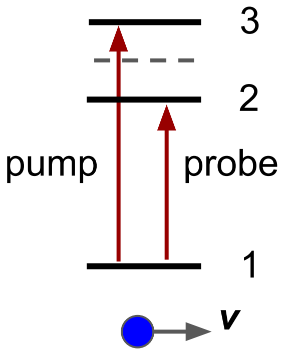
^{85}Rb D1 line (F=2)



$kv_z = (\omega_{12} - \omega_{13})/2:$



$kv_z = (\omega_{13} - \omega_{12})/2:$

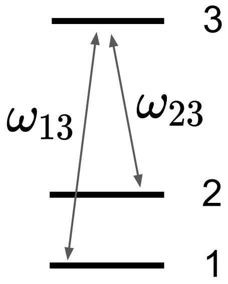


For atoms resonant with the probe light:

- pump de-populates the ground state
- →less absorption

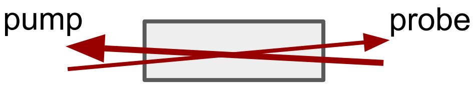
SAS Crossover Resonances (Ground State)

3-level “Λ”



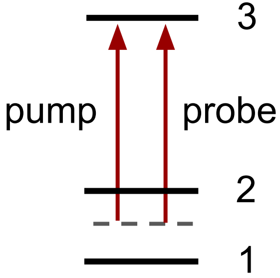
Counter-propagating beams with

$$\omega = (\omega_{23} + \omega_{13})/2$$

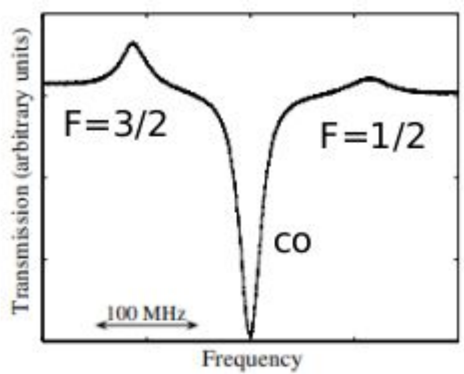


Atoms Doppler-shifted into resonance:

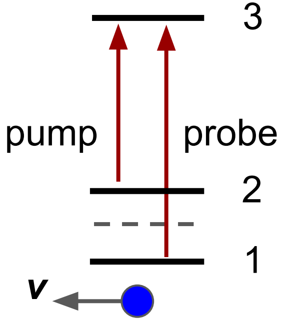
$$v_z = 0 :$$



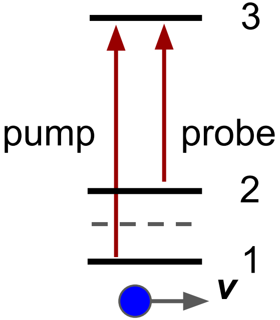
^{6}Li D2 line



$$kv_z = (\omega_{23} - \omega_{13})/2 :$$



$$kv_z = (\omega_{13} - \omega_{23})/2 :$$



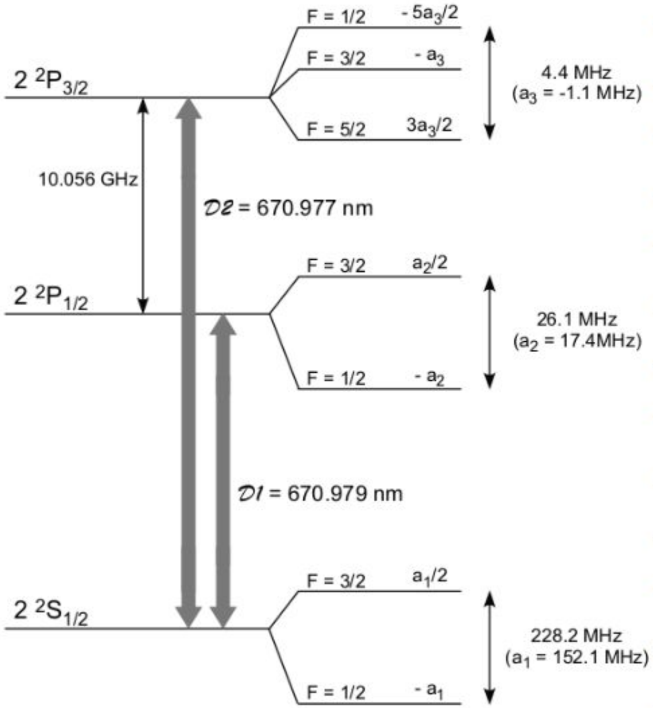
For atoms resonant with the probe light:

- pump populates the probed ground state
- →more absorption

SAS Example 4: ^{6}Li

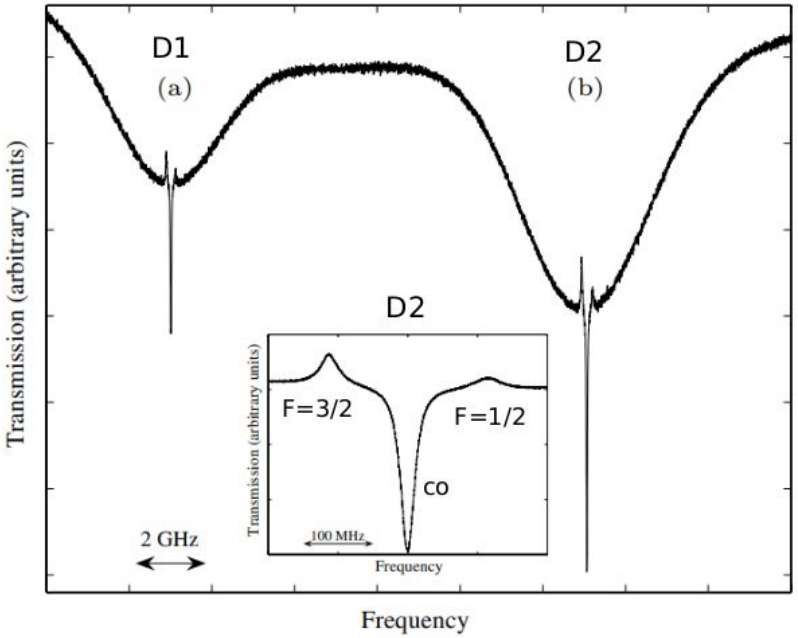
^{6}Li D1 & D2 Lines ($\Gamma = 5.8$ MHz)

$$\Delta\omega_D \approx 2\pi \times 3.3\,\mathrm{GHz}$$



M. Gehm, "Properties of 6Li"

Ground-state crossover features (Li-6)



Fuchs et al, J. Phys. B: At. Mol. Opt. Phys. 39, 3479 (2006)