Thursday, April 4, 2024

(I) Fine structure Hamiltonian (continued)

$$H_{LS} = \frac{1}{2}\frac{e^2}{m_e^2 c^2}\frac{1}{R^3}\vec{L}\cdot\vec{S} = E_{LS}\,\vec{L}\cdot\vec{S}$$

$$= \frac{E_{LS}}{2}\left(\vec{J}^2 - \vec{L}^2 - \vec{S}^2\right)$$

vector-operator

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

$\Rightarrow \vec{J}^2 = \vec{L}^2 + \vec{S}^2 + 2\vec{L}\cdot\vec{S}$

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

possible values for J: $J = L+S,\ L+S-1,\ \ldots,\ |L-S|$

Example: For $L=1$, $S=1/2$ $\Rightarrow$ $J = 3/2$ or $1/2$

$$\Rightarrow H_{LS} = \frac{E_{LS}}{2}\left[J(J+1) - \underbrace{L(L+1)}_{2} - \underbrace{S(S+1)}_{3/4}\right]$$

$$= \frac{E_{LS}}{2}\begin{cases} 3/4 - 2 - 3/4 = -2 & \text{for } J = 1/2 \\ \frac{15}{4} - 2 - 3/4 = 1 & \text{for } J = 3/2 \end{cases}$$

II Hyperfine Hamiltonian

(see E. Arimondo, M. Inguscio, and P. Violino, RMP 49, 31 (1977))

The nuclear spin $\vec{I}$ interacts with the angular momentum of the electron, which yields a Hamiltonian

$$H_{hyperfine} = hA\,\vec{I}\cdot\vec{J} + hB\,\frac{6(\vec{I}\cdot\vec{J})^2 + 3(\vec{I}\cdot\vec{J}) - 2I(I+1)J(J+1)}{2I(2I-1)\,2J(2J-1)}$$

A = hyperfine A coefficient → due to nuclear magnetic dipole moment

B = hyperfine B coefficient → due to electric quadrupole moment of the nucleus

For an S-level, B = 0 and we get

$$H_{hyperfine} = \frac{16\pi}{3}\,\frac{\mu_0}{4\pi}\,\mu_B^2\, g_I\, |\psi_s(0)|\, \underbrace{\vec{I}\cdot\vec{S}}_{\frac{1}{2}(\vec{F}^2 - \vec{I}^2 - \vec{S}^2)}$$

$\vec{F} = \vec{I} + \vec{J}$ = total angular momentum of atom

One can show that (with $K = F(F+1) - I(I+1) - J(J+1)$)

$$E_{HFS} = \frac{hA}{2}K + hB\,\frac{\frac{3}{2}K(K+1) - 2I(I+1)J(J+1)}{2I(2I-1)2J(J-1)}$$

Zeeman substructure

The interaction of the atom with an external $\vec{B}$-field is given by:

positive is 1.4 MHz/G

$$H_{Zeeman} = +\frac{\mu_B}{\hbar}\left[g_S \underset{S_z}{\vec{S}} + g_L \underset{L_z}{\vec{L}} + g_I \underset{I_z}{\vec{I}} \right] \cdot \underset{B_z}{\vec{B}}$$

where $g_L = 1 - \frac{m_e}{m_{nucleus}} \simeq 1$

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

↳ $\hat{z}$ = quantization axis

$$g_S = 2.\underbrace{002319304362}_{\text{9 digits of agreement with QED theory}} \simeq 2$$

g_I = nuclear g-factor $\simeq -9.95141 \times 10^{-4}$ for Rb 87

$$\mu_B = \frac{e\hbar}{2m_e} = +9.27408 \times 10^{-24}\ J/T = +1.4\ MHz/G$$

If the Zeeman energy shift is small compared to the fine structure splitting, then according to perturbation theory

very small

$$E(J, m_J) = \langle J, m_J | H_{Zeeman} | J, m_J \rangle = -\frac{\mu_B}{\hbar}\left(g_J J_z + g_I I_z\right) B_z$$

with the Landé factor g_J given by

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

for $g_s = 2$, $g_L = 1$, then $g_J = 1 + \dfrac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$

setting $g_I = 0$, we can see this in the following manner

$$E(J, m_J) = \langle J, m_J | H_{Zeeman} | J, m_J \rangle$$

$$= \langle J, m_J | + \frac{\mu_B}{\hbar} (\vec{L} + 2\vec{S}) \cdot \vec{B} | J, m_J \rangle$$

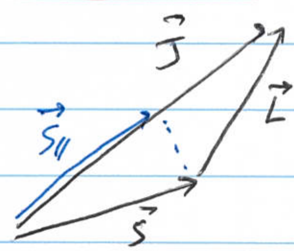
$$= \langle J, m_J | + \frac{\mu_B}{\hbar} (\vec{J} + \vec{S}) \cdot \vec{B} | J, m_J \rangle$$

The $\{|J, m_J\rangle\}$ basis forms a subspace in the larger space spanned by the $\{|L, m_L\rangle \otimes |S, m_s\rangle\}$ basis.

The Wigner-Eckart Projection theorem states

$$\boxed{\langle J, m_J | \vec{S} | J, m_J \rangle = \frac{\langle J, m_J | \vec{J} \cdot \vec{S} | J, m_J \rangle}{\langle J, m_J | \vec{J}^2 | J, m_J \rangle} \vec{J} = \vec{S}_{\parallel}}$$

Geometric picture :



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

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

Thus $E(J, m_J) = \langle J, m_J | + \dfrac{\mu_B}{\hbar} \vec{J} \cdot \vec{B} | J, m_J \rangle + \dfrac{\mu_B}{\hbar} \dfrac{\langle J, m_J | \vec{J} \cdot \vec{S} | J, m_J \rangle \langle J, m_J | \vec{J} \cdot \vec{B} | J, m_J \rangle}{\langle J, m_J | \vec{J}^2 | J, m_J \rangle}$

$$E(J,m_J) = \frac{\mu_B}{\hbar} \langle J, m_J | \left(1 + \frac{1}{2} \frac{J(J+1) + S(S+1) - L(L+1)}{J(J+1)} \right) \vec{J} \cdot \vec{B} \,|\, J, m_J \rangle$$

If the Zeeman Energy shift is small compared to the Hyperfine splitting, then we can write

$$H_{Zeeman} = \frac{\mu_B}{\hbar} g_F \, \vec{F} \cdot \vec{B} = \mu_B g_F m_F B_z$$

with the hyperfine Lande g-factor given by

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

very small