Helium $2\,{}^3P_2 \rightarrow 5\,{}^3D_j$ coupling

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1 Basis states

1.1 Field-free eigenstates

The atomic helium system is best represented using the LS coupling scheme. Because of the 1s electron, the L quantum number is both the total orbital angular momentum and the 2nd electron orbital angular momentum. The S angular moment is:

$$\boldsymbol{S} = \boldsymbol{S}_1 + \boldsymbol{S}_2. \tag{1}$$

In addition, the spin-orbit coupling means that L_z and S_z do not commute with the Hamiltonian, and we then need

$$\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S} \tag{2}$$

instead. This leads us to the following set of quantum numbers to describe a state:

$$|\alpha\rangle \equiv |1snlLSJm_J\rangle \equiv |nLSJm_J\rangle \equiv n\,{}^{2S+1}L_J \tag{3}$$

where the RHS is the simplified notation, written in a term symbol.

These states are eigenstates of the system in the absence of a magnetic field. Hence, we can write:

$$H_0 = T + V \tag{4}$$

and

$$H_0|nLSJm_J\rangle = E(n\,{}^{2S+1}L_J) \tag{5}$$

which is independent of m_J.

1.2 Zeeman shift

The magnetic field Hamiltonian, for a magnetic field oriented along z, i.e. $\boldsymbol{B} = B\hat{\boldsymbol{z}}$ is:

$$H_B = -\mu_z B \tag{6}$$

where

$$\mu_z = \frac{-\mu_B}{\hbar}(g_l L_z + g_s S_z) \tag{7}$$

where $g_L = 1$ and $g_S \approx 2$. Hence, this operator does not commute with H_0 and does not commute with $\hat{J}^2$ or $\hat{J}_z$. The closest basis to $|\alpha\rangle$ which is an eigenstate of μ_z is:

$$|\beta\rangle \equiv |nLm_LSm_S\rangle. \tag{8}$$

Because $|\alpha\rangle$ and $|\beta\rangle$ share many quantum numbers, these with be indicated with $\gamma = \{1snlLS\}$ for simplicity. That is:

$$|\alpha\rangle \equiv |\gamma Jm_J\rangle \tag{9}$$

and

$$|\beta\rangle \equiv |\gamma m_L m_S\rangle \tag{10}$$

The action of H_B in $|\beta\rangle$ is:

$$H_B|\gamma m_L m_S\rangle = \frac{-\mu_B}{\hbar}B(m_L + 2m_S) \tag{11}$$

Note that this commutes with $\hat{J}_z$ but not $\hat{J}^2$. So we could also write this as:

$$\begin{aligned} H_B|\gamma m_L m_S\rangle &= \frac{-\mu_B}{\hbar}B(m_L + 2(m_J - m_L)) && (12)\\ &= \frac{-\mu_B}{\hbar}B(2m_J - m_L) && (13) \end{aligned}$$

2 Coupling between bases

The coupling between the $|\alpha\rangle$ and $|\beta\rangle$ bases is given by the Clebsch-Gordan coefficients. I will just state the result:

$$|\gamma J m_J\rangle = \sum_{m_L m_S} C^{LSJ}_{m_L m_S m_J}|\gamma m_L m_S\rangle. \tag{14}$$

For $L = 2$ and $S = 1$, (i.e. the $5\ ^3D_j$ manifold), we can represent these as a vector.

$$\boldsymbol{\alpha} = \begin{bmatrix}|1-1\rangle & \cdots & |11\rangle & |2-2\rangle & \cdots & |22\rangle & |3-3\rangle & \cdots & |33\rangle\end{bmatrix}^T \tag{15}$$

(note: $J = 0$ is forbidden, due to the triangle relationship, i.e. $|L-S| \leq J \leq L+S$) and

$$\boldsymbol{\beta} = \begin{bmatrix}|-2-1\rangle & \cdots & |2-1\rangle & |-20\rangle & \cdots & |20\rangle & |-21\rangle & \cdots & |21\rangle\end{bmatrix}^T \tag{16}$$

(note, same number of states between $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$) and then the Clebsch-Gordan coefficients will make up a unitary matrix:

$$\boldsymbol{\alpha} = U\boldsymbol{\beta} \tag{17}$$

This matrix will be very sparse. It only connects states where $m_L + m_S = m_J$. As we are only interested in the final states, where $m_J = 1$ because of the σ^- coupling, we can restrict ourselves to:

$$\boldsymbol{\alpha} = \begin{bmatrix}|11\rangle & |21\rangle & |31\rangle\end{bmatrix}^T \tag{18}$$

and

$$\boldsymbol{\beta} = \begin{bmatrix}|01\rangle & |10\rangle & |2-1\rangle\end{bmatrix}^T. \tag{19}$$

In this combination, the matrix U looks like:

$$\begin{bmatrix} 0.316228 & -0.547723 & 0.774597 \\ -0.707107 & 0.408248 & 0.57735 \\ 0.632456 & 0.730297 & 0.258199 \end{bmatrix} \tag{20}$$

which would definitely have a nicer representation using surds, but I can't be bothered looking these up.

3 Hamiltonian

I will assume that the only things we can detect are differences in energy. Hence, I will place the $j = 3$ state at $E_3 = 0$ and vary E_2. For E_1 I will assume $E_1 = 315$ MHz.

The Hamiltonian matrix elements are then:

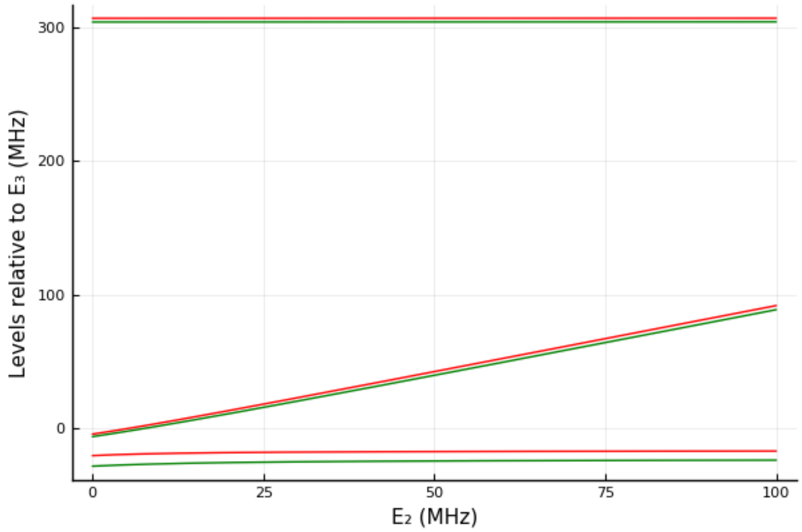
$$\boldsymbol{\alpha}^T H_0 \boldsymbol{\alpha} = \begin{bmatrix} 315\,\text{MHz} & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{21}$$

and

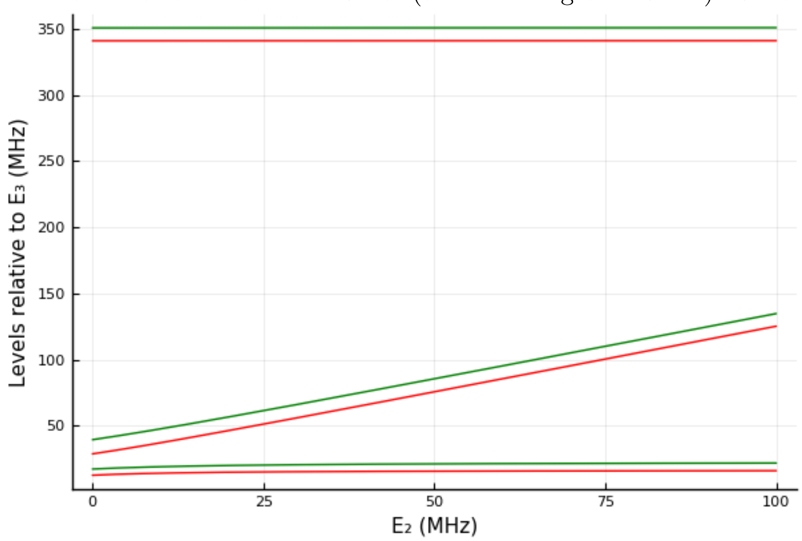
$$\begin{aligned} \boldsymbol{\alpha}^T H_B \boldsymbol{\alpha} &= \boldsymbol{\beta}^T U^T H_B U \boldsymbol{\beta} && (22)\\ &= \frac{-\mu_B}{\hbar} B U^T \begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} U && (23)\\ &= \frac{-\mu_B}{\hbar} B \begin{bmatrix} 0.7 & -0.635085 & 0.0816497 \\ -0.635085 & 0.766667 & -0.612826 \\ 0.0816497 & -0.612826 & 1.53333 \end{bmatrix} && (24) \end{aligned}$$

4 Results

After working out the eigenvalues, remembering that $E_3 = 0$ in the presence of the field, I find the following (red = 8 Gauss and green = 11 Gauss)



I also plotted the same, but with the shift due to the magnetic field on the $2\ ^3P_2$, $m_J = 2$ level. This will be a constant shift for all of the red curves (as with the green curves) but it will different between the red/green pairs.



Note: there doesn't seem to be any indication of three levels! What could be going wrong? Also... the levels seem a lot further apart than in the draft.