Untangling hyperfine level malarkey

1 Context

Figure 1 shows absorption peaks for laser light to helium at frequencies denoted by the x-axis in a DC magnetic field of strength 11G and 18G (blue and red respectively). The atom is initially in the $m_J = 2$ state of the 2^3P_2 level.

These lines are identified as transitions to the 5^3D_2 and 5^3D_3 levels. We also have measured frequencies for the $2^3P_2 \to 5^3D_1$ transition in both background fields. The problem statement is: *Given* the experimentally measured peak frequencies and *assuming* the quantum mechanical description of the atom, *determine* the absolute frequencies of the $2^3P_2 \to 5_D$ transitions in the unperturbed helium atom. The outcome is currently a partial solution, and an indication of what is needed to reach a more complete solution.

1.1 Old method

Previously, I used a linear fit to the peak values as a function of field strength to extrapolate to the zero-field values. This isn't horrifically wrong but it is incorrect because for small field values, there is a nonlinear shift in the closely-spaced energies of the D_2 and D_3 levels, as explained below. Therefore one must use Actual Theory to work obtain the field-free transition energies.

I asked Danny for some assistance here, and what follows is an extension of the background material he provided.

2 Identifing peaks

Figure 2 shows the frequencies of the transitions to the $J = 2$ and $J = 3$ levels, relative to the zero-field $J = 3$ level, as a function of field strength assuming a 21MHz splitting between the bare levels. Shown are the $m_j = 1$ (black), 2 (blue), and 3 (red) lines from each level (the $J = 3$ being the lowest). Notice that at 11G and 18G, the experimentally relevant fields, the $|J, m_J\rangle = |3, 2\rangle$ and $|J, m_J\rangle = |2, 1\rangle$ lines are very close, or even intersecting. In the red spectrum in figure 1, one can just make out two distinct peaks in the central peak. We conclude that the larger central peak in both spectra is the coincidence of the two transitions. Checking the metadata for this experimental run confirms that the waveplate was set at an angle such that some π light was present, which is different from the other measured spectra (not shown here).

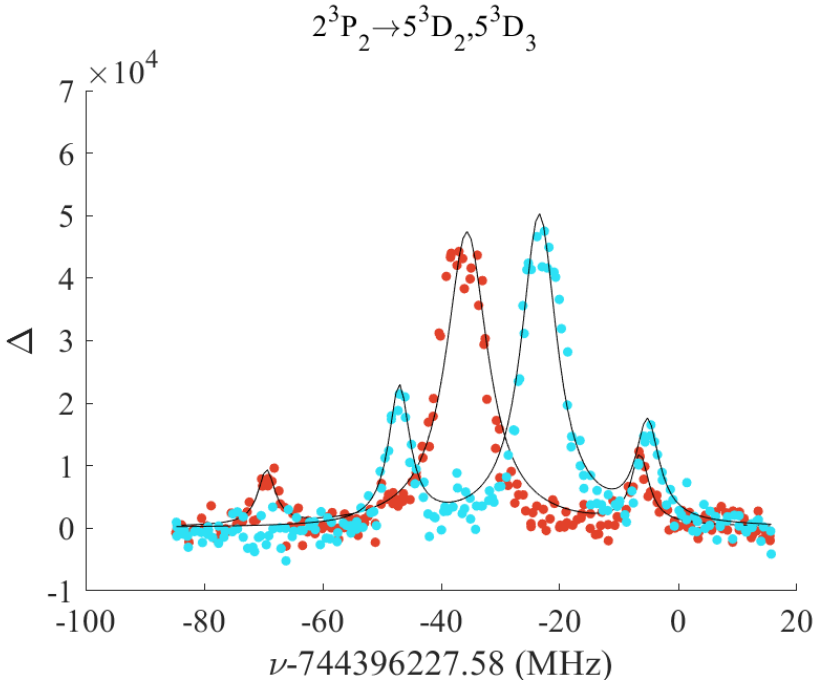

Figure 1: Beautiful peaks, look at them shine

The question now is to determine the zero-field value of the fine structure splitting. We will use the smaller extremal peaks, the $|J, m_J\rangle = |3, 1\rangle$ and $|J, m_J\rangle = |2, 2\rangle$ lines, for this calculation as they are sufficiently distinct. The peak separation depends on the zero-field splitting and the magnetic field strength. By fixing the latter we can constrain the former. By minimizing the squared difference between the predicted and measured interval $f_{|3,1\rangle} - f_{|2,2\rangle}$, we constrain the splitting. Figure 2b. shows the squared error as a function of splitting value, which is minimized at 21MHz, 2MHz larger than the 19MHz prediction given in Wiese and Fuhr.

This does not, unfortunately, give us the absolute frequency of these levels. In this calculation, the $J = 1 - J = 3$ interval was assumed to be 315 MHz (actually larger than the predicted 303MHz, but the interference from a peak this far away should be small). In the next part I suggest a few ways forward.

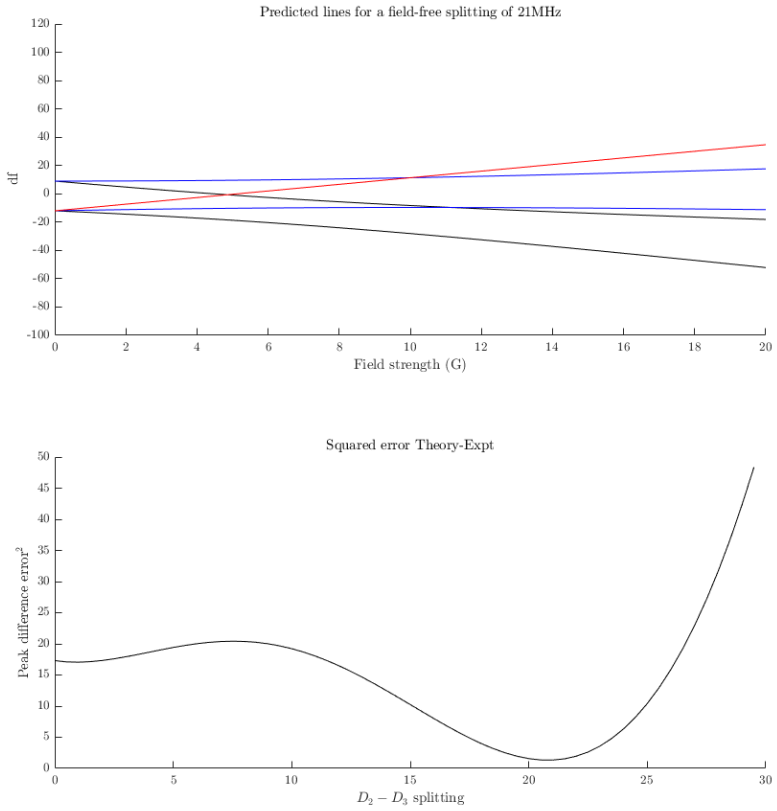

Figure 2: Theoretical lines as a function of magnetic field strength for fixed splitting, and the sum-square error of the predicted $f_{|3,1\rangle} - f_{|2,2\rangle}$, summed over measurements at both field values, versus the fine structure splitting.

3 Determination of the absolute transition frequencies

The current methods allow us to determine the fine structure splitting between the $J = 2$ and $J = 3$ levels of the helium 5^3D manifold (Are those terms right?). Determining the absolute frequency will require additional intervals. Up until now, the $J = 3 - J = 1$ interval was input to the calculations. This is circular, assuming the theory we are trying to test. We would do better to use our experimental data and the quantum theory of the atom to work backwards to the field intervals. We could do this by extending the treatment above with a three-parameter fit - the absolute frequency of the $J = 1$ transition, and the fine structure intervals (or, equivalently, the absolute frequencies of each transition), fitting to all available peaks as listed in table **??**.

4 Extending work

Whereas previously we just used the CG coefficients givin the $\langle Jm_J|$ basis in terms of the $\langle m_L m_S|$ basis, using only the $m_J = 1$ subspace, we now need to extend this to the $m_J = 2$ and $m_J = 3$ subspace. This is just a matter of writing some bigger matrices, but involves calculating/looking up more CG coefficients.

(remember the $|\alpha\rangle$ basis is the $|Jm_J\rangle$ basis and the $|\beta\rangle$ basis is the $|m_L m_S\rangle$ basis.)

So we want to work in the subspace spanned by

$$\boldsymbol{\alpha} = \{|11\rangle, |21\rangle, |12\rangle, |31\rangle, |32\rangle\} \tag{1}$$

We also have one (bad) measurement which includes the $|33\rangle$ line but we don't talk about that.

What's the basis we want to project back on to, then? The $|\beta\rangle$ basis, subject to $m_L + m_S = m_J$. In the upper state, $L = 2$ so $m_L \in \{-2, -1, 0, 1, 2\}$ and $m_S \in \{-1, 0, 1\}$ right? and $m_J \in \{1, 2\}$.

$$\boldsymbol{\alpha} = \{|01\rangle, |10\rangle, |2-1\rangle, |11\rangle, |20\rangle\} \tag{2}$$

Ok great, now just need to look up the CG coefficients! And can look at Danny's work to confirm. U transforms the $m_L m_S$ basis into the Jm_J basis.

U is:

$$\begin{bmatrix} \sqrt{1/10} & -\sqrt{3/10} & \sqrt{3/5} & 0 & 0 \\ -\sqrt{1/2} & \sqrt{1/6} & \sqrt{1/3} & 0 & 0 \\ \sqrt{2/5} & \sqrt{8/15} & \sqrt{1/15} & 0 & 0 \\ & 0 & 0 & -\sqrt{1/3} & \sqrt{2/3} \\ & 0 & 0 & \sqrt{2/3} & \sqrt{1/3} \end{bmatrix} \tag{3}$$

Helium $2\,{}^3P_2 \to 5\,{}^3D_j$ 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:

$$|\beta\rangle \equiv |nLm_L Sm_S\rangle. \tag{8}$$

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:

$$H_B|\gamma m_L m_S\rangle = \frac{-\mu_B}{\hbar} B(m_L + 2(m_J - m_L)) \tag{12}$$

$$= \frac{-\mu_B}{\hbar} B(2m_J - m_L) \tag{13}$$

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

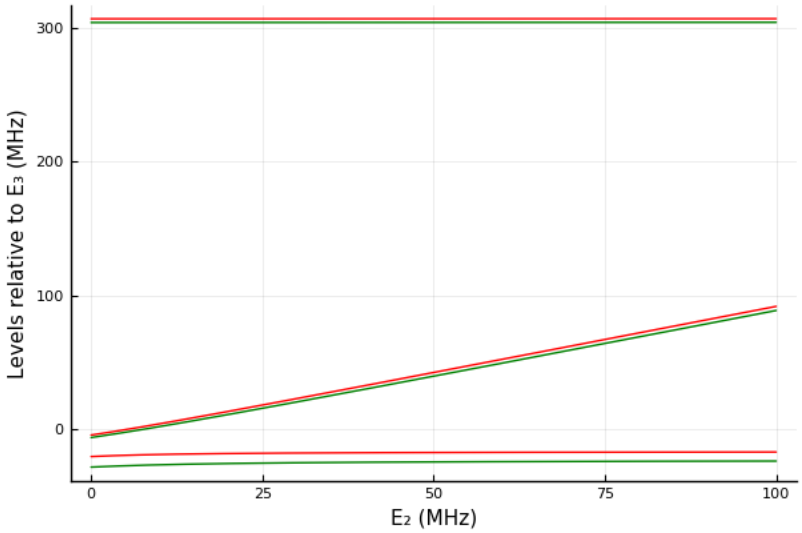
$$\boldsymbol{\alpha}^T H_B \boldsymbol{\alpha} = \boldsymbol{\beta}^T U^T H_B U \boldsymbol{\beta} \tag{22}$$

$$= \frac{-\mu_B}{\hbar} B U^T \begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} U \tag{23}$$

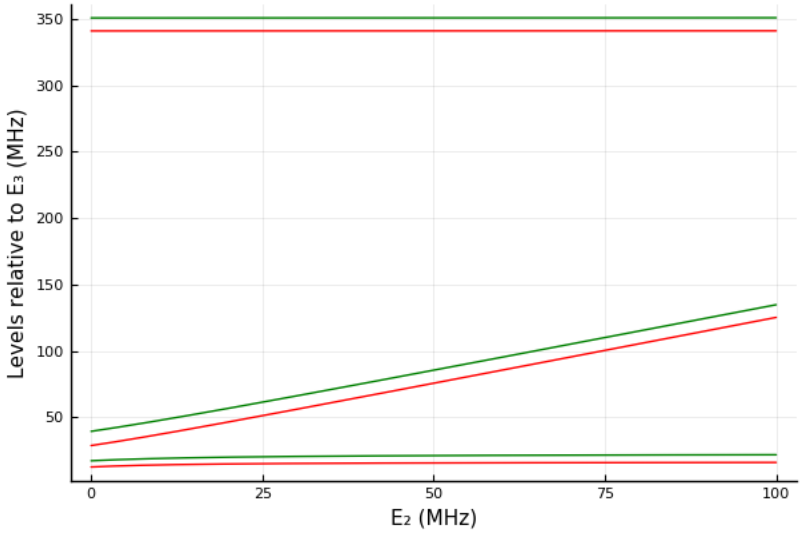
$$= \frac{-\mu_B}{\hbar} B \begin{bmatrix} 0.7 & -0.635085 & 0.0816497 \\ -0.635085 & 0.766667 & -0.612826 \\ 0.0816497 & -0.612826 & 1.53333 \end{bmatrix} \tag{24}$$

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.

Line	Field	Peak centre	peak width
5^3D_1	$\|B\| = 18G$	744396451.51(0.10) MHz	6.43(0.29) MHZ
	$\|B\| = 11G$	744396475.92(0.12) MHz	5.15(0.33) MHZ
$5^3D_{2,3}$	$\|B\| = 18G$	744396158.56(0.21) MHz	3.44(0.55) MHZ
		744396191.07(0.16) MHz	8.56(0.49) MHZ
		744396221.11(0.16) MHz	3.67(0.44) MHZ
	$\|B\| = 11G$	744396180.50(0.14) MHz	4.34(0.40) MHZ
		744396204.54(0.13) MHz	7.33(0.39) MHZ
		744396222.65(0.16) MHz	4.75(0.47) MHZ

Table 1: Relevant measured peak frequencies