The problem

An electron is in an $\ell = 1$ state of a hydrogen atom. It experience a spin orbit interaction

$$V_{so} = \alpha \vec{L} \cdot \vec{S}$$

and feels an external magnetic field

$$V_b = \mu \vec{B} \cdot \left(\vec{L} + 2\vec{S} \right)$$

Calculate the eigenvalues of the Hamiltonian in the $|JM\rangle$ basis.

Outline - steps to solve the problem

1. Calculate Clebsch–Gordan coefficients to obtain a change of basis matrix C which transforms from $|m_\ell, m_s\rangle$ to the $|JM\rangle$ basis
2. Write $V_{so}^{(J)}$ in terms of operators $\vec{J}^2$, $\vec{L}^2$, and $\vec{S}^2$
3. Calculate matrix elements of the spin-orbit term $V_{so}^{(J)}$
4. Write $V_b^{(\ell s)}$ in terms of operators L_z and S_z
5. Calculate matrix elements of $V_b^{(\ell s)}$
6. Use the matrix C from step one to transform $V_b^{(\ell s)}$ to $V_b^{(J)}$
7. Write out the matrix $H = V_{so}^{(J)} + V_b^{(J)}$ and calculate the eigenvalues of the 6x6 matrix

Calculate the Clebsch-Gordan coefficients

Some useful operators:

$$J_-|J,M\rangle = \hbar\sqrt{(J+M)(J-M+1)}|J,M-1\rangle$$

$$S_-|s,m_s\rangle = \hbar\sqrt{(s+m_s)(s-m_s+1)}|s,m_s-1\rangle$$

$$L_-|\ell,m_\ell\rangle = \hbar\sqrt{(\ell+m_\ell)(\ell-m_\ell+1)}|\ell,m_\ell-1\rangle$$

$$J_- = S_- + L_-$$

Calculate the Clebsch-Gordan coefficients

Begin at the top of the ladder. There is only one $|m_\ell, m_s\rangle$ state corresponding to the $|J, M\rangle$ state with $M = \ell + s$.

$$\boxed{\left|J = \frac{3}{2}, M = \frac{3}{2}\right\rangle = \left|m_\ell = 1, m_s = \frac{1}{2}\right\rangle}$$

Calculate the Clebsch-Gordan coefficients

Apply the lowering operator to obtain the coefficients for the state with the same J, but with $M = \ell + s - 1$.

$$J_- \left| J = \frac{3}{2}, M = \frac{3}{2} \right\rangle = (S_- + L_-) \left| m_\ell = 1, m_s = \frac{1}{2} \right\rangle$$

$$\hbar\sqrt{3} \left| J = \frac{3}{2}, M = \frac{1}{2} \right\rangle = \hbar \left| m_\ell = 1, m_s = -\frac{1}{2} \right\rangle + \hbar\sqrt{2} \left| m_\ell = 0, m_s = \frac{1}{2} \right\rangle$$

$$\boxed{\left| J = \frac{3}{2}, M = \frac{1}{2} \right\rangle = \sqrt{\frac{1}{3}} \left| m_\ell = 1, m_s = -\frac{1}{2} \right\rangle + \sqrt{\frac{2}{3}} \left| m_\ell = 0, m_s = \frac{1}{2} \right\rangle}$$

Calculate the Clebsch-Gordan coefficients

$$\boxed{\left|J=\frac{3}{2},M=\frac{1}{2}\right\rangle=\sqrt{\frac{1}{3}}\left|m_\ell=1,m_s=-\frac{1}{2}\right\rangle+\sqrt{\frac{2}{3}}\left|m_\ell=0,m_s=\frac{1}{2}\right\rangle}$$

Since there are two possible $|m_\ell, m_s\rangle$ states corresponding to $|J=3/2, M=1/2\rangle$, there must be another $|JM\rangle$ state expressed as a linear combination of the same $|m_\ell, m_s\rangle$ orthogonal to that above, with $J=\ell+s-1$ (switch the coefficients and make one negative).

$$\boxed{\left|J=\frac{1}{2},M=\frac{1}{2}\right\rangle=\sqrt{\frac{2}{3}}\left|m_\ell=1,m_s=-\frac{1}{2}\right\rangle-\sqrt{\frac{1}{3}}\left|m_\ell=0,m_s=\frac{1}{2}\right\rangle}$$

This multiplet must begin at the top of its own ladder.

Calculate the Clebsch-Gordan coefficients

Going further gives states with negative M, which mirror those we've already calculated.

$$\boxed{\left|J=\frac{3}{2},M=-\frac{1}{2}\right\rangle=\sqrt{\frac{1}{3}}\left|m_\ell=-1,m_s=\frac{1}{2}\right\rangle+\sqrt{\frac{2}{3}}\left|m_\ell=0,m_s=-\frac{1}{2}\right\rangle}$$

$$\boxed{\left|J=\frac{1}{2},M=-\frac{1}{2}\right\rangle=\sqrt{\frac{2}{3}}\left|m_\ell=-1,m_s=\frac{1}{2}\right\rangle-\sqrt{\frac{1}{3}}\left|m_\ell=0,m_s=-\frac{1}{2}\right\rangle}$$

$$\boxed{\left|J=\frac{3}{2},M=-\frac{3}{2}\right\rangle=\left|m_\ell=-1,m_s=-\frac{1}{2}\right\rangle}$$

No new multiplets are opened because the number of $|m_\ell, m_s\rangle$ states per level doesn't increase.

Create a transformation matrix

We can use all these relations to form a matrix that transforms an $|m_\ell, m_s\rangle$ state into a $|JM\rangle$ state.

$$\begin{pmatrix} \left|\frac{3}{2},\frac{3}{2}\right\rangle \\ \left|\frac{3}{2},\frac{1}{2}\right\rangle \\ \left|\frac{1}{2},\frac{1}{2}\right\rangle \\ \left|\frac{3}{2},-\frac{1}{2}\right\rangle \\ \left|\frac{1}{2},-\frac{1}{2}\right\rangle \\ \left|\frac{3}{2},-\frac{3}{2}\right\rangle \end{pmatrix} = \begin{pmatrix} 1 & & & & & \\ & \sqrt{\frac{1}{3}} & \sqrt{\frac{2}{3}} & & & \\ & \sqrt{\frac{2}{3}} & -\sqrt{\frac{1}{3}} & & & \\ & & & \sqrt{\frac{1}{3}} & \sqrt{\frac{2}{3}} & \\ & & & \sqrt{\frac{2}{3}} & -\sqrt{\frac{1}{3}} & \\ & & & & & 1 \end{pmatrix} \begin{pmatrix} \left|1,\frac{1}{2}\right\rangle \\ \left|1,-\frac{1}{2}\right\rangle \\ \left|0,\frac{1}{2}\right\rangle \\ \left|-1,\frac{1}{2}\right\rangle \\ \left|0,-\frac{1}{2}\right\rangle \\ \left|-1,-\frac{1}{2}\right\rangle \end{pmatrix}$$

$$|\psi^{(J)}\rangle = C\,|\psi^{(\ell s)}\rangle$$

Since the coefficients are real:

$$C^T = C^{-1}$$

Calculate the spin-orbit term

$$V_{so} = \alpha \vec{L} \cdot \vec{S}$$

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

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

There is only J-dependence so the matrix is diagonal in the $|JM\rangle$ basis.

Calculate the spin-orbit term

$$\left\langle J=\frac{3}{2}, M=\frac{3}{2}\middle| V_{so} \middle| J=\frac{3}{2}, M=\frac{3}{2}\right\rangle = \left\langle \frac{3}{2}, \frac{1}{2}\middle| V_{so} \middle| \frac{3}{2}, \frac{1}{2}\right\rangle =$$

$$\left\langle \frac{3}{2}, -\frac{1}{2}\middle| V_{so} \middle| \frac{3}{2}, -\frac{1}{2}\right\rangle = \left\langle \frac{3}{2}, -\frac{3}{2}\middle| V_{so} \middle| \frac{3}{2}, -\frac{3}{2}\right\rangle = \frac{\alpha\hbar^2}{2}$$

$$\left\langle \frac{1}{2}, \frac{1}{2}\middle| V_{so} \middle| \frac{1}{2}, \frac{1}{2}\right\rangle = \left\langle \frac{1}{2}, -\frac{1}{2}\middle| V_{so} \middle| \frac{1}{2}, -\frac{1}{2}\right\rangle = -\alpha\hbar^2$$

$$V_{so}^{(J)} = \frac{\alpha\hbar^2}{2}\begin{pmatrix} 1 & & & & & \\ & 1 & & & & \\ & & -2 & & & \\ & & & 1 & & \\ & & & & -2 & \\ & & & & & 1 \end{pmatrix}$$

Calculate the Zeeman term

$$V_b = \mu \vec{B} \cdot \left(\vec{L} + 2\vec{S} \right)$$

$$\left\langle m_\ell = 1, m_s = \frac{1}{2} \middle| V_b \middle| m_\ell = 1, m_s = \frac{1}{2} \right\rangle = 2\mu\hbar B$$

$$\left\langle 1, -\frac{1}{2} \middle| V_b \middle| 1, -\frac{1}{2} \right\rangle = 0 \qquad \left\langle 0, \frac{1}{2} \middle| V_b \middle| 0, \frac{1}{2} \right\rangle = \mu\hbar B$$

$$\left\langle -1, \frac{1}{2} \middle| V_b \middle| -1, \frac{1}{2} \right\rangle = 0 \qquad \left\langle 0, -\frac{1}{2} \middle| V_b \middle| 0, -\frac{1}{2} \right\rangle = -\mu\hbar B$$

$$\left\langle -1, -\frac{1}{2} \middle| V_b \middle| -1, -\frac{1}{2} \right\rangle = -2\mu\hbar B$$

Calculate the Zeeman term

This term is diagonal in the $|m_\ell, m_s\rangle$ basis.

$$V_b^{(\ell s)} = \mu\hbar B \begin{pmatrix} 2 & & & & & \\ & 0 & & & & \\ & & 1 & & & \\ & & & 0 & & \\ & & & & -1 & \\ & & & & & -2 \end{pmatrix}$$

We perform a transformation to the $|JM\rangle$ basis using the matrix of Clebsch-Gordan coefficients.

Calculate the Zeeman term

$$V_b^{(J)} = CV_b^{(\ell s)}C^T = \mu\hbar B \begin{pmatrix} 2 & & & & & \\ & \frac{2}{3} & -\frac{\sqrt{2}}{3} & & & \\ & -\frac{\sqrt{2}}{3} & \frac{1}{3} & & & \\ & & & -\frac{2}{3} & \frac{\sqrt{2}}{3} & \\ & & & \frac{\sqrt{2}}{3} & -\frac{1}{3} & \\ & & & & & -2 \end{pmatrix}$$

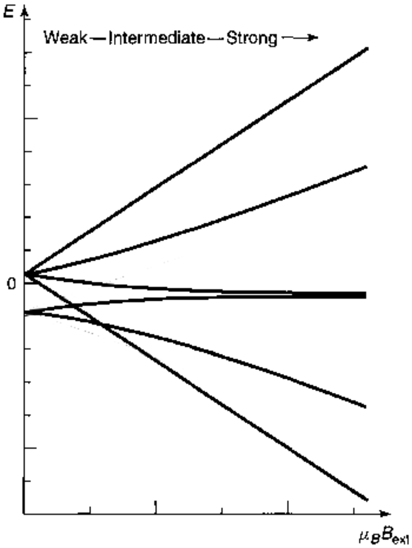
Write down the Hamiltonian

$$H^{(J)} = V_{so}^{(J)} + V_b^{(J)}$$

$$= \begin{pmatrix} \frac{\alpha\hbar^2}{2} + 2\mu\hbar B & & & & & \\ & \frac{\alpha\hbar^2}{2} + \frac{2}{3}\mu\hbar B & -\frac{\sqrt{2}}{3}\mu\hbar B & & & \\ & -\frac{\sqrt{2}}{3}\mu\hbar B & -\alpha\hbar^2 + \frac{1}{3}\mu\hbar B & & & \\ & & & \frac{\alpha\hbar^2}{2} - \frac{2}{3}\mu\hbar B & \frac{\sqrt{2}}{3}\mu\hbar B & \\ & & & \frac{\sqrt{2}}{3}\mu\hbar B & -\alpha\hbar^2 - \frac{1}{3}\mu\hbar B & \\ & & & & & \frac{\alpha\hbar^2}{2} - 2\mu\hbar B \end{pmatrix}$$

Calculate the eigenvalues

$$E = \begin{cases} \frac{\alpha\hbar^2}{2} \pm 2\mu\hbar B \\ \frac{\mu\hbar B}{2} - \frac{\alpha\hbar^2}{4} \pm \sqrt{\left(\frac{\alpha\hbar^2}{4} + \frac{\mu\hbar B}{2}\right)^2 + \frac{\alpha^2\hbar^4}{2}} \\ -\frac{\mu\hbar B}{2} - \frac{\alpha\hbar^2}{4} \pm \sqrt{\left(\frac{\alpha\hbar^2}{4} - \frac{\mu\hbar B}{2}\right)^2 + \frac{\alpha^2\hbar^4}{2}} \end{cases}$$


E
Weak — Intermediate — Strong →
0
$\mu_B B_{ext}$