E&M II - Project 2 Calculations.

The **Zeeman effect** is an effect that comes about from putting an atom in a magnetic field. The magnetic field causes a magnetic moment to be produced and perturbs the energy levels of the atom causing spectral line shifts to appear when modeled or measured with spectroscopy.

Hydrogen Atom First Order Magnetic Field Energy Corrections

To begin, the unperturbed wave functions of hydrogen is given by

$$H^{(0)} = \underbrace{\frac{\vec{p}^2}{2m}}_{\text{Kinetic term}} - \underbrace{\frac{\hbar c \alpha}{r}}_{\text{Potential term}}. \tag{1}$$

Consider the atom now in a magnetic field $\vec{B}$. The electrons spin will yield a magnetic moment $\vec{\mu}_S = \frac{-eg_s}{2m}\vec{S}$. The energy interaction of a single magnetic moment $\vec{\mu}$ with a fixed external magnetic field is given by $H^\mu = -\mu \cdot \vec{B}$ and so the Hamiltonian change due to this effect is $H_S^{(1)} = -\mu_s \cdot \vec{B} = \frac{eg_s}{2m}\vec{S} \cdot \vec{B}$. There is also a correction due to the angular momentum of the electron. If we assume that the electron is moving in a circle, then this has a magnetic dipole $\mu_L = \frac{-e}{2m}\vec{L}$ and so there exists another correction to the Hamiltonian $H_L^{(1)} = -\mu_L \cdot \vec{B} = \frac{eg_L}{2m}\vec{L} \cdot \vec{B}$. Now, g_s is a bi-products of the Dirac equation has a value of $g_s = s$. Combining these terms together give the total Zeeman effect to the Hamiltonian $H_{magnetic}^{(1)}$,

$$H_{magnetic}^{(1)} \equiv H_{mag}^{(1)} = \frac{e}{2m}(\vec{L} + 2\vec{S}) \cdot \vec{B} = \frac{\mu_B}{\hbar}(\vec{L} + 2\vec{S}) \cdot \vec{B}, \tag{2}$$

where $\mu_B = \frac{e\hbar}{2m}$ is the Bohr magneton.

If we are just considering the changes that come about from the Zeeman effect, we can ignore other Hamiltonian perturbations such as the fine structure and hyperfine structure interactions. Assume that $\vec{B} \equiv B\hat{z}$ then the Hamiltonian will only contain z components after performing the dot product giving $H_{mag}^{(1)} = \frac{\mu_B}{\hbar}(L_z + 2S_z)B$. Now, $\vec{J} = \vec{L} + \vec{S} \implies L_z = J_z - S_z$ and so $H_{mag}^{(1)} = \frac{\mu_B}{\hbar}(J_z + S_z)B$. From perturbation theory we can solve for the first order energy corrections to this using

$$\begin{aligned} E_n^{(1)} &= \langle njm_j\ell s|H_{mag}^{(1)}|njm_j\ell s\rangle \\ &= \frac{\mu_B B}{\hbar}\langle njm_j\ell s|(J_z + S_z)|njm_j\ell s\rangle \\ &= \frac{\mu_B B}{\hbar}\left(\hbar m_j + \langle njm_j\ell s|S_z|njm_j\ell s\rangle\right). \end{aligned} \tag{3}$$

We can determine S_z by projecting $\vec{S}$ onto $\vec{J}$ which gives $\vec{S} = \frac{\vec{J}\cdot\vec{S}}{\vec{J}^2}\vec{J}$ and then using the substitution that

$$\vec{J} \cdot \vec{S} = (\vec{L} + \vec{S}) \cdot \vec{S} = \vec{L} \cdot \vec{S} + \vec{S}^2 = \frac{1}{2}(\vec{J}^2 - \vec{L}^2 - \vec{S}^2) + \vec{S}^2 = \frac{1}{2}(\vec{J}^2 - \vec{L}^2 + \vec{S}^2). \tag{4}$$

This, we have

$$S_z = \frac{(\vec{J}^2 - \vec{L}^2 + \vec{S}^2)}{2\vec{J}^2}J_z, \tag{5}$$

and so the undetermined matrix element in (3) becomes

$$
\begin{aligned}
\langle njm_j\ell s|S_z|njm_j\ell s\rangle &= \langle njm_j\ell s|\frac{(\vec{J}^2 - \vec{L}^2 + \vec{S}^2)}{2\vec{J}^2}J_z|njm_j\ell s\rangle \\
&= m_j\hbar\frac{j(j+1) - \ell(\ell+1) + s(s+1)}{2j(j+1)}.
\end{aligned}
\tag{6}
$$

Plugging this back into (3) gives us

$$
\boxed{E_n^{(1)} = \mu_B B m_j\left[1 + \frac{j(j+1) - \ell(\ell+1) + s(s+1)}{2j(j+1)}\right] = \mu_B B m_j g_L},
\tag{7}
$$

where g_L is the Landé g factor

$$
g_L = 1 + \frac{j(j+1) - \ell(\ell+1) + s(s+1)}{2j(j+1)}.
\tag{8}
$$

References

[1] Our brains.