Note on the Zeeman Effect

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1 One Electron Atom

Consider the interaction between an electron and a uniform magnetic field $\boldsymbol{B}$. This field can be derived from the vector potential

$$\boldsymbol{A} = \frac{1}{2}\,[\boldsymbol{B} \times \boldsymbol{r}]$$

The interaction Hamiltonian is

$$h_{\rm int}(r) = -ec\;\boldsymbol{\alpha}\cdot\boldsymbol{A} = -\frac{ec}{2}\;\boldsymbol{\alpha}\cdot[\boldsymbol{B}\times\boldsymbol{r}] = -\frac{ec}{2}\;\boldsymbol{B}\cdot[\boldsymbol{r}\times\boldsymbol{\alpha}]$$

We may rewrite the cross product on the right side of this equation as

$$[\boldsymbol{r}\times\boldsymbol{\alpha}]_\lambda = -i\sqrt{2}\,r\left(\boldsymbol{\alpha}\cdot\boldsymbol{C}^{(0)}_{1\lambda}(\hat{r})\right)$$

Assuming $\boldsymbol{B}$ is in the z direction, the interaction becomes

$$h_{\rm int}(r) = i\frac{ecB}{2}\sqrt{2}\,r\left(\boldsymbol{\alpha}\cdot\boldsymbol{C}^{(0)}_{10}(\hat{r})\right)$$

The interaction energy W_v in a valence state $|v\rangle$ of a one electron atom may be written

$$W_v = \langle v|h_{\rm int}|v\rangle = i\frac{ecB}{2}\sqrt{2}\,\left\langle v\left|\left(\boldsymbol{\alpha}\cdot\boldsymbol{C}^{(0)}_{10}(\hat{r})\right)\right|v\right\rangle$$

The matrix element of $\boldsymbol{\alpha}\cdot\boldsymbol{C}^{(0)}_{10}$ above is

$$\begin{aligned}
-\,i\int_0^\infty dr\,r\,P_v(r)Q_v(r)\,\Big[&\left\langle\kappa_v m_v\left|\left(\boldsymbol{\sigma}\cdot\boldsymbol{C}^{(0)}_{10}(\hat{r})\right)\right|-\kappa_v m_v\right\rangle \\
&-\left\langle-\kappa_v m_v\left|\left(\boldsymbol{\sigma}\cdot\boldsymbol{C}^{(0)}_{10}(\hat{r})\right)\right|\kappa_v m_v\right\rangle\Big] \\
&= i\left\langle-\kappa_v m_v\left|\left(\boldsymbol{\sigma}\cdot\boldsymbol{C}^{(0)}_{10}(\hat{r})\right)\right|\kappa_v m_v\right\rangle (r)_{vv}
\end{aligned}$$

where

$$(r)_{vv} = 2\int_0^\infty dr\,r\,P_v(r)Q_v(r).$$

We note that

$$\left\langle -\kappa_v m_v \left| \left(\boldsymbol{\sigma} \cdot \boldsymbol{C}_{10}^{(0)}(\hat{r}) \right) \right| \kappa_v m_v \right\rangle = \frac{2\kappa_v}{\sqrt{2}} \langle -\kappa_v m_v | C_0^1(\hat{r}) | \kappa_v m_v \rangle.$$

Therefore, we have

$$W_v = \frac{ec}{2} \, B(-2\kappa_v) \langle -\kappa_v m_v | C_0^1(\hat{r}) | \kappa_v m_v \rangle (r)_{vv}$$

It is simple to show that

$$\langle -\kappa_v m_v | C_0^1(\hat{r}) | \kappa_v m_v \rangle = -\frac{m_v}{2j_v(j_v+1)}$$

Moreover, in the Pauli approximation,

$$\begin{aligned} (r)_{vv} = & -\frac{1}{c} \int_0^\infty dr \, r \, P_v \left(\frac{dP_v}{dr} + \frac{\kappa_v}{r} P_v \right) \\ & = -\frac{1}{c} \int_0^\infty dr \left(\frac{1}{2} \frac{dr P_v^2}{dr} + \frac{1}{2} (2\kappa_v - 1) P_v^2 \right) = -\frac{2\kappa_v - 1}{2c} \end{aligned}$$

Putting this together, we obtain the following expression for the interaction energy:

$$W_v = -\mu_B B \, g_v m_v, \qquad (1)$$

where

$$g_v = \frac{\kappa_v(2\kappa_v - 1)}{j_v(j_v+1)} = \frac{2j_v + 1}{2l_v + 1}$$

is the Landé g-factor of the atomic term, and

$$\mu_B = \frac{e\hbar}{2m} \equiv \frac{e}{2}$$

is the Bohr magneton.

2 Comparison with Classical Result

The interaction energy of a classical current $\boldsymbol{j} = e\boldsymbol{v}$ with a magnetic field is

$$W = -\boldsymbol{j} \cdot \boldsymbol{A} = -\frac{e}{2} \, \boldsymbol{v} \cdot [\boldsymbol{B} \times \boldsymbol{r}] = -\frac{e\hbar}{2m} \, \boldsymbol{B} \cdot \boldsymbol{L} = -\mu_B B \, L_0$$

with angular momentum $\boldsymbol{L}$ expressed in units of $\hbar$. The quantum mechanical version of this result would be

$$W_v = -\mu_B B \, \langle v m_v | L_0 | v m_v \rangle$$

To understand our result in terms of the classical picture, we replace $\boldsymbol{L}$ by a linear combination of $\boldsymbol{L}$ and $\boldsymbol{S}$:

$$\boldsymbol{L} \to g_L \boldsymbol{L} + g_S \boldsymbol{S}$$

Thus, we we are led consider

$$W_v = -\mu_B B \, \langle v | g_L L_0 + g_S S_0 | v \rangle. \tag{2}$$

To evaluate the above matrix elements, we make use of a result that is valid for any tensor operator $\boldsymbol{V}$ of rank 1:

$$\langle jm | V_0 | jm \rangle = \frac{\langle jm | \boldsymbol{J} \cdot \boldsymbol{V} | jm \rangle}{j(j+1)} \, m.$$

From this equation, we find that

$$\begin{aligned} \langle v m_v | L_0 | v m_v \rangle &= \frac{j_v(j_v+1) + l_v(l_v+1) - s(s+1)}{2 j_v (j_v+1)} \, m_v \\ &= \begin{cases} \dfrac{2j_v - 1}{2l_v + 1} \, m_v, & j_v = l_v + 1/2 \\ \dfrac{2j_v + 3}{2l_v + 1} \, m_v, & j_v = l_v - 1/2 \end{cases} \end{aligned}$$

and

$$\begin{aligned} \langle v m_v | S_0 | v m_v \rangle &= \frac{j_v(j_v+1) - l_v(l_v+1) + s(s+1)}{2 j_v (j_v+1)} \, m_v \\ &= \begin{cases} \dfrac{1}{2l_v + 1} \, m_v, & j_v = l_v + 1/2 \\ -\dfrac{1}{2l_v + 1} \, m_v, & j_v = l_v - 1/2 \end{cases} \end{aligned}$$

Choosing $g_L = 1$ and $g_S = 2$ in Eq.(**??**), we obtain presicely the quantum mechanical result given in Eq.(**??**):

$$W_v = -\mu_e B \, g_v m_v,$$

with

$$g_v = \frac{2j_v + 1}{2l_v + 1}$$