Zeeman effect (theory)

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Here we discuss the Zeeman effect using the perturbation theory. The discussion here consists of three parts, depending on the magnitude of magnetic field; (i) in the weak magnetic field limit where the spin-orbit interaction H_{so} is dominant: (i) the intermediate magnetic field where the spin-orbit interaction is comparable with the Zeeman energy, and (iii) the strong magnetic field where the Zeeman energy H_B is dominant.

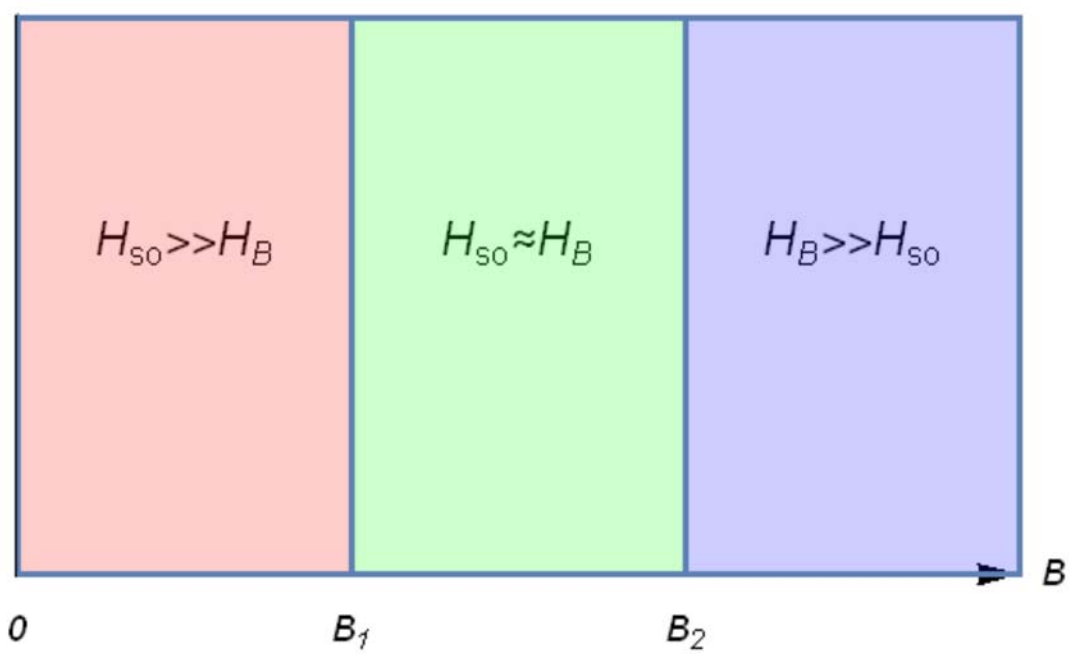
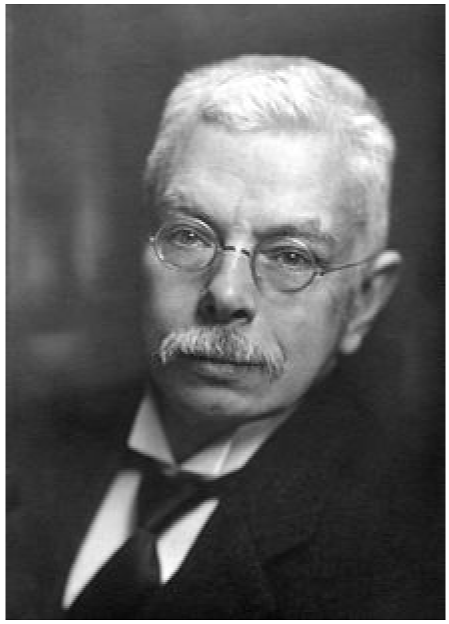


Fig. H_{so} is the spin-orbit interaction. H_B is the Zeeman energy.

((**Pieter Zeeman**))



Pieter Zeeman (25 May 1865 – 9 October 1943) was a Dutch physicist who shared the 1902 Nobel Prize in Physics with Hendrik Lorentz for his discovery of the Zeeman effect.

((**Alfred Landé**))
Alfred Landé (13 December 1888–30 October 1976) was a German-American physicist known for his contributions to quantum theory. He is responsible for the Landé *g*-factor and an explanation of the Zeeman Effect.

http://en.wikipedia.org/wiki/Alfred_Land%C3%A9

1. Orbital magnetic moment and spin magnetic moment

The total angular momentum $\boldsymbol{J}$ is defined by

$$\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S} .$$

The total magnetic moment $\boldsymbol{\mu}$ is given by

$$\boldsymbol{\mu} = -\frac{\mu_B}{\hbar}(\boldsymbol{L} + 2\boldsymbol{S}) .$$

The total magnetic moment along the direction of J, $\boldsymbol{\mu}_J$, is defined by

$$\boldsymbol{\mu}_J = -\frac{g_J \mu_B}{\hbar}\boldsymbol{J} ,$$

where g_J is the Lande g-factor.

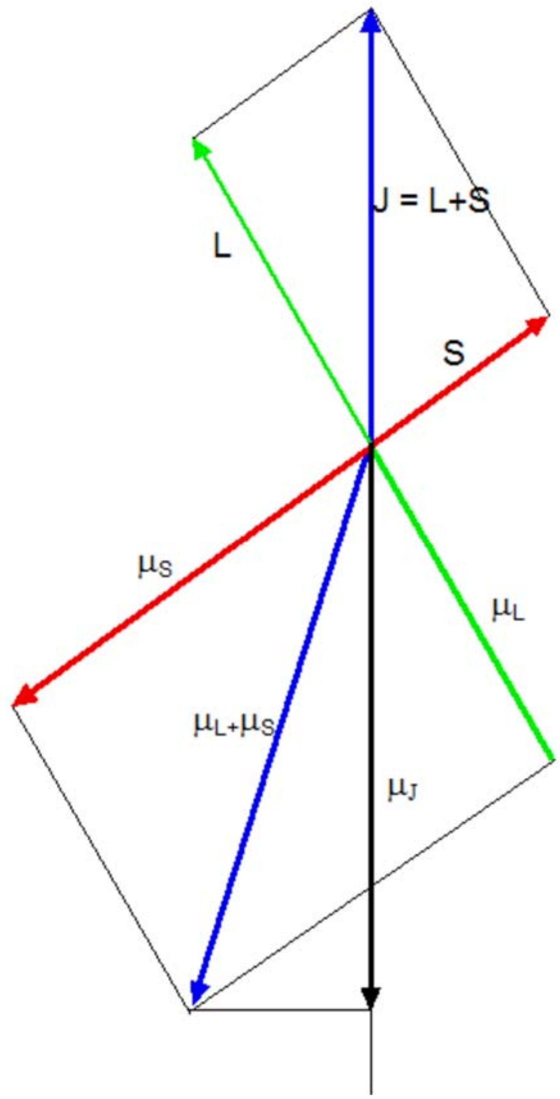


Fig. Basic classical vector model of orbital angular momentum (***L***), spin angular momentum (***S***), orbital magnetic moment ($\boldsymbol{\mu}_L$), and spin magnetic moment ($\boldsymbol{\mu}_S$). ***J*** (= ***L*** + ***S***) is the total angular momentum. $\boldsymbol{\mu}_J$ is the component of the total magnetic moment ($\boldsymbol{\mu}_L + \boldsymbol{\mu}_S$) along the direction (-***J***).

Suppose that

$$\boldsymbol{L} = a\boldsymbol{J} + \boldsymbol{L}_\perp \text{ and } \boldsymbol{S} = b\boldsymbol{J} + \boldsymbol{S}_\perp,$$

where *a* and *b* are constants, and the vectors $\mathbf{S}_\perp$ and $\mathbf{L}_\perp$ are perpendicular to ***J***.

Here we have the relation $a+b=1$, and $\boldsymbol{L}_\perp + \boldsymbol{S}_\perp = 0$. The values of a and b are determined as follows.

$$a = \frac{\boldsymbol{J}\cdot\boldsymbol{L}}{\boldsymbol{J}^2}, \; b = \frac{\boldsymbol{J}\cdot\boldsymbol{S}}{\boldsymbol{J}^2}.$$

Here we note that

$$\boldsymbol{J}\cdot\boldsymbol{S} = (\boldsymbol{L}+\boldsymbol{S})\cdot\boldsymbol{S} = \boldsymbol{S}^2 + \boldsymbol{L}\cdot\boldsymbol{S} = \boldsymbol{S}^2 + \frac{\boldsymbol{J}^2 - \boldsymbol{L}^2 - \boldsymbol{S}^2}{2} = \frac{\boldsymbol{J}^2 - \boldsymbol{L}^2 + \boldsymbol{S}^2}{2},$$

or

$$\boldsymbol{J}\cdot\boldsymbol{S} = \frac{\boldsymbol{J}^2 - \boldsymbol{L}^2 + \boldsymbol{S}^2}{2} = \frac{\hbar^2}{2}[J(J+1) - L(L+1) + S(S+1)],$$

using the average in quantum mechanics. The total magnetic moment $\boldsymbol{\mu}$ is

$$\boldsymbol{\mu} = -\frac{\mu_B}{\hbar}(\boldsymbol{L}+2\boldsymbol{S}) = -\frac{\mu_B}{\hbar}[(a+2b)\boldsymbol{J} + (L_\perp + 2S_\perp)].$$

Thus we have

$$\boldsymbol{\mu}_J = -\frac{\mu_B}{\hbar}(a+2b)\boldsymbol{J} = -\frac{\mu_B}{\hbar}(1+b)\boldsymbol{J} = -\frac{g_J\mu_B}{\hbar}\boldsymbol{J},$$

with

$$g_J = 1 + b = 1 + \frac{\boldsymbol{J}\cdot\boldsymbol{S}}{\boldsymbol{J}^2} = \frac{3}{2} + \frac{s(s+1) - L(L+1)}{2J(J+1)}.$$

2. Derivation of Landé *g*-factor: approach from the classical model

In the classical theory, the projection vectors of the spin angular momentum $\boldsymbol{S}$ and the orbital angular momentum $\boldsymbol{L}$ along the direction of the total angular momentum J

$$\boldsymbol{S}_J = \frac{\boldsymbol{S}\cdot\boldsymbol{J}}{|\boldsymbol{J}|^2}\boldsymbol{J}, \qquad \boldsymbol{L}_J = \frac{\boldsymbol{L}\cdot\boldsymbol{J}}{|\boldsymbol{J}|^2}\boldsymbol{J},$$

where

$$\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}.$$

The total magnetic moment along the direction of $\boldsymbol{J}$ is given by

$$\boldsymbol{\mu}_J = -\frac{\mu_B}{\hbar}\left(\frac{\boldsymbol{L}\cdot\boldsymbol{J}}{|\boldsymbol{J}|^2}\boldsymbol{J} + 2\frac{\boldsymbol{S}\cdot\boldsymbol{J}}{|\boldsymbol{J}|^2}\boldsymbol{J}\right).$$

Using $\boldsymbol{L} = \boldsymbol{J} - \boldsymbol{S}$, and squaring both sides, we get

$$\boldsymbol{L}^2 = \boldsymbol{J}^2 + \boldsymbol{S}^2 - 2\boldsymbol{J}\cdot\boldsymbol{S},$$

or

$$\boldsymbol{J}\cdot\boldsymbol{S} = \frac{\boldsymbol{J}^2 + \boldsymbol{S}^2 - \boldsymbol{L}^2}{2}.$$

Using $\boldsymbol{S} = \boldsymbol{J} - \boldsymbol{L}$, and squaring both sides, we get

$$\boldsymbol{S}^2 = \boldsymbol{J}^2 + \boldsymbol{L}^2 - 2\boldsymbol{J}\cdot\boldsymbol{L},$$

or

$$\boldsymbol{J}\cdot\boldsymbol{L} = \frac{\boldsymbol{J}^2 + \boldsymbol{L}^2 - \boldsymbol{S}^2}{2}.$$

Then we get

$$\boldsymbol{\mu}_J = -\frac{\mu_B}{\hbar \boldsymbol{J}^2}(\boldsymbol{L}\cdot\boldsymbol{J} + 2\boldsymbol{S}\cdot\boldsymbol{J})\boldsymbol{J}$$
$$= -\frac{\mu_B}{2\hbar \boldsymbol{J}^2}[\boldsymbol{J}^2 + \boldsymbol{L}^2 - \boldsymbol{S}^2 + 2(\boldsymbol{J}^2 + \boldsymbol{S}^2 - \boldsymbol{L}^2)]\boldsymbol{J}$$
$$= -\frac{\mu_B}{\hbar}\frac{(3\boldsymbol{J}^2 - \boldsymbol{L}^2 + \boldsymbol{S}^2)}{2\boldsymbol{J}^2}\boldsymbol{J}$$

The Landé g-factor is defined by

$$g_J = \frac{(3\boldsymbol{J}^2 - \boldsymbol{L}^2 + \boldsymbol{S}^2)}{2\boldsymbol{J}^2} = \frac{3}{2} + \frac{\boldsymbol{S}^2 - \boldsymbol{L}^2}{2\boldsymbol{J}^2}.$$

In quantum mechanics, we get

$$g_J = \frac{3}{2} + \frac{s(s+1) - l(l+1)}{2j(j+1)},$$

using the relations, $\boldsymbol{J}^2 \to \hbar^2 j(j+1)$, $\boldsymbol{S}^2 \to \hbar^2 s(s+1)$, and $\boldsymbol{L}^2 \to \hbar^2 L(L+1)$. The total magnetic moment is given by

$$\boldsymbol{\mu}_J = -\frac{\mu_B}{\hbar} g_j \boldsymbol{J}.$$

3. Derivation of Landé *g*-factor: approach from the Wigner-Eckhart

The specific formula we need from the Wigner-Eckhart theorem relates the matrix element of any general vector component $\hat{V}_z$ to the matrix element of the total magnetic momentum. $\hat{J}_z$;

$$\langle jm|\hat{V}_z|jm'\rangle = \frac{\langle j||\hat{\boldsymbol{V}}\cdot\hat{\boldsymbol{J}}||jm\rangle}{\hbar^2 j(j+1)}\langle jm|\hat{J}_z|jm'\rangle.$$

For the Zeeman effect, ***L*** or ***S*** play the role of the vector ***V***. This equation is called the projection theorem because of the role of the projection ***V.J*** in determining the constant of proportionality between the matrix of V_z and J_z. Note that the matrix element of the projection ***V.J*** is a diagonal element, but the V_z and J_z matrix elements are general matrix elements between different *m* states within a given *j* subspace.

$$\langle j || \hat{\boldsymbol{S}} \cdot \hat{\boldsymbol{J}} || j \rangle = \frac{1}{2} \langle j || \hat{\boldsymbol{J}}^2 + \hat{\boldsymbol{S}}^2 - \hat{\boldsymbol{L}}^2 || j \rangle$$
$$= \frac{\hbar^2}{2} [j(j+1) + s(s+1) - l(l+1)]$$

and

$$\langle j || \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{J}} || jm \rangle = \frac{1}{2} \langle j || \hat{\boldsymbol{J}}^2 + \hat{\boldsymbol{L}}^2 - \hat{\boldsymbol{S}}^2 || j \rangle$$
$$= \frac{\hbar^2}{2} [j(j+1) + l(l+1) - s(s+1)]$$

Then we have

$$\langle jm | \hat{S}_z | jm' \rangle = \frac{\langle j || \hat{\boldsymbol{S}} \cdot \hat{\boldsymbol{J}} || j \rangle}{\hbar^2 j(j+1)} \langle jm | \hat{J}_z | jm' \rangle$$
$$= \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)} \langle jm | \hat{J}_z | jm' \rangle$$

$$\langle jm | \hat{L}_z | jm' \rangle = \frac{\langle j || \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{J}} || j \rangle}{\hbar^2 j(j+1)} \langle jm | \hat{J}_z | jm' \rangle$$
$$= \frac{j(j+1) + l(l+1) - s(s+1)}{2j(j+1)} \langle jm | \hat{J}_z | jm' \rangle$$

The total magnetic moment along the z axis is given by

$$\hat{\mu}_z = -\frac{\mu_B}{\hbar} (\hat{L}_z + 2\hat{S}_z) .$$

Then we have

$$
\begin{aligned}
\langle jm|\hat{L}_z + 2\hat{S}_z|jm'\rangle &= \\
&= [\frac{j(j+1)+l(l+1)-s(s+1)}{2j(j+1)} \\
&\quad + \frac{j(j+1)+s(s+1)-l(l+1)}{j(j+1)}]\langle jm|\hat{J}_z|jm'\rangle \\
&= [\frac{3}{2} + \frac{s(s+1)-l(l+1)}{2j(j+1)}]\langle jm|\hat{J}_z|jm'\rangle \\
&= g_J\langle jm|\hat{J}_z|jm'\rangle
\end{aligned}
$$

where g_J is the Landé g-factor given by

$$g_J = \frac{3}{2} + \frac{s(s+1)-l(l+1)}{2j(j+1)}.$$

Then magnetic moment is given by

$$\hat{\mu}_z = -\frac{\mu_B}{\hbar}(\hat{L}_z + 2\hat{S}_z) = -\frac{\mu_B}{\hbar}g_J\hat{J}_z.$$

4. Zeeman effect in the weak magnetic field

In the presence of the magnetic field B along the z axis, the Zeeman energy is given by

$$\hat{H}_B = \frac{g_J\mu_B B}{\hbar}\hat{J}_z.$$

The first-order Zeeman energy correction:

$$E_B^{(1)} = \langle jm|\hat{H}_B|jm\rangle = \frac{g_J\mu_B B}{\hbar}\langle jm|\hat{J}_z|jm\rangle = g_J m\mu_B B.$$

For $j = l + \frac{1}{2}$, $s = \frac{1}{2}$,

$$g_J = \frac{3}{2} + \frac{\frac{3}{4} - l(l+1)}{2j(j+1)} = 1 + \frac{1}{2l+1},$$

$$E_B^{(1)} = m(1+\frac{1}{2l+1})\mu_B B.$$

For $j = l - \frac{1}{2}$,

$$g_J = \frac{3}{2} + \frac{\frac{3}{4} - l(l+1)}{2j(j+1)} = 1 - \frac{1}{2l+1},$$

$$E_B^{(1)} = m(1-\frac{1}{2l+1})\mu_B B.$$

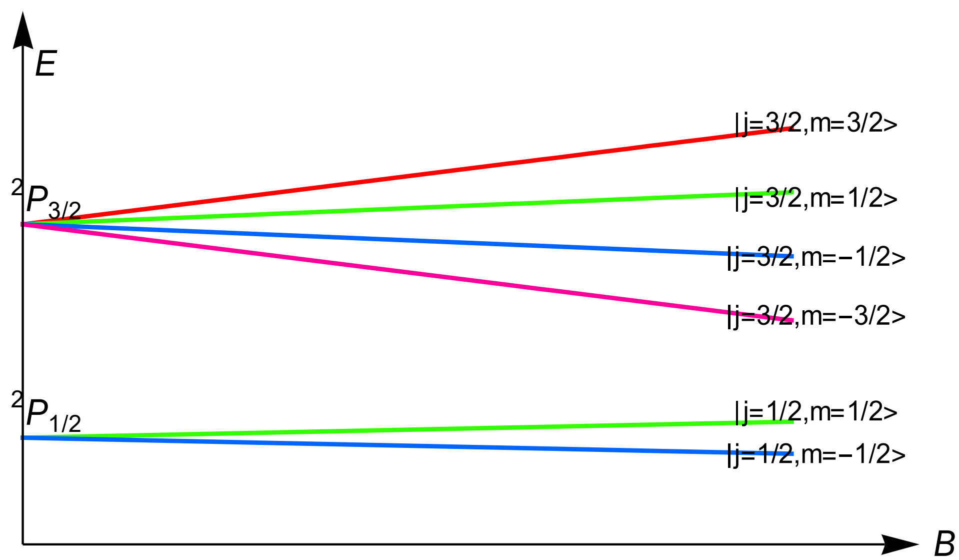
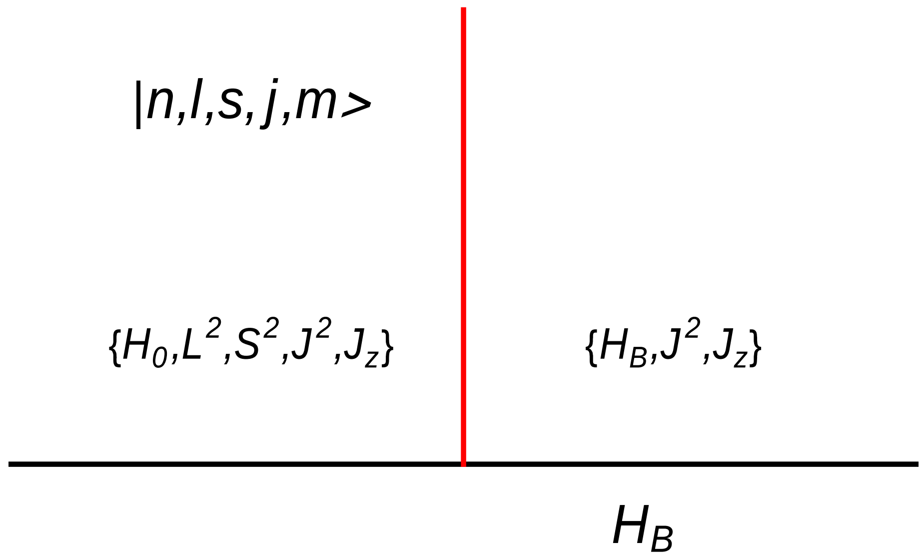


Fig. Weak-field Zeeman structure of the hydrogen 2 P fine structure levels labeled with the quantum numbers of the coupled basis states. $n = 2$. $j = 3/2$ and $j = 1/2$. $l = 1$ and $s = 1/2$. The splitting of the levels between $^2P_{3/2}$ and $^2P_{1/2}$ at $B = 0$ is due to the spin orbit interaction.



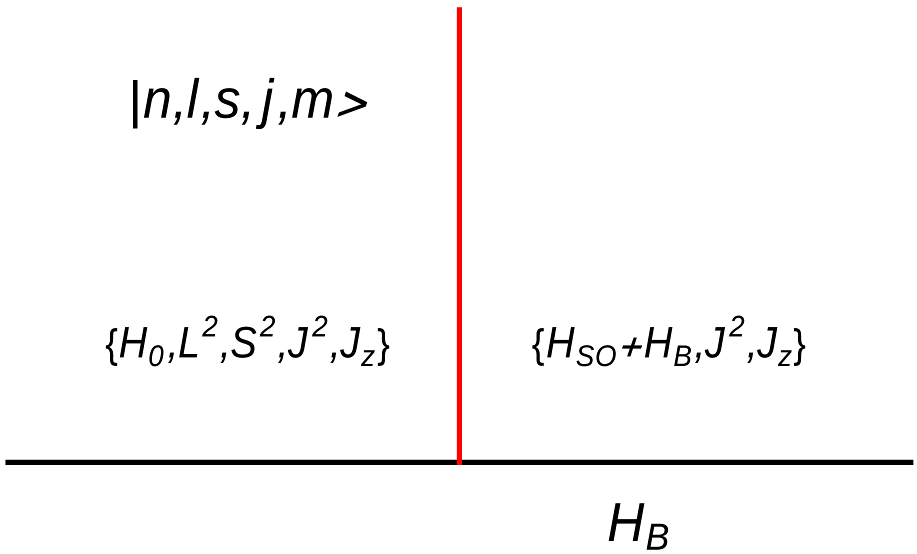
5. Zeeman effect in the intermediate magnetic field

In the presence of magnetic field along the z axis, the Zeeman energy is given by

$$\hat{H}_B = -\hat{\boldsymbol{\mu}} \cdot \boldsymbol{B} = \frac{\mu_B}{\hbar}(\hat{\boldsymbol{L}} + 2\hat{\boldsymbol{S}}) \cdot \boldsymbol{B} = \frac{\mu_B}{\hbar}(\hat{\boldsymbol{J}} + \hat{\boldsymbol{S}}) \cdot \boldsymbol{B} = \frac{\mu_B B}{\hbar}(\hat{J}_z + \hat{S}_z) .$$

The perturbed Hamiltonian is the sum of the spin orbit interaction $\hat{H}_{so}$ and the Zeeman energy $\hat{H}_B$ as

$$\hat{H}_1 = \hat{H}_{so} + \hat{H}_B = \frac{\xi\hbar^2}{2}\frac{1}{\hbar^2}\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}} + \mu_B B \frac{1}{\hbar}(L_z + 2S_z) .$$



Note that $\hat{H}_{so}$ is comparable to $\hat{H}_B$. The matrix of $\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}$ under the basis of $\left|\phi_1\right\rangle = \left|m_l = m-\frac{1}{2}, m_s = \frac{1}{2}\right\rangle$ and $\left|\phi_2\right\rangle = \left|m_l = m+\frac{1}{2}, m_s = -\frac{1}{2}\right\rangle$, is obtained as

$$\frac{2}{\hbar^2}\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}} = \begin{pmatrix} (m-\frac{1}{2}) & \sqrt{(l+m+\frac{1}{2})(l-m+\frac{1}{2})} \\ \sqrt{(l+m+\frac{1}{2})(l-m+\frac{1}{2})} & -(m+\frac{1}{2}) \end{pmatrix}.$$

We note that

$$\frac{1}{\hbar}(L_z + 2S_z)\left|m_l = m-\frac{1}{2}, m_s = \frac{1}{2}\right\rangle = (m+\frac{1}{2})\left|m_l = m-\frac{1}{2}, m_s = \frac{1}{2}\right\rangle,$$

$$\frac{1}{\hbar}(L_z + 2S_z)\left|m_l = m+\frac{1}{2}, m_s = -\frac{1}{2}\right\rangle = (m-\frac{1}{2})\left|m_l = m-\frac{1}{2}, m_s = \frac{1}{2}\right\rangle.$$

So the matrix of $\frac{1}{\hbar}(L_z + 2S_z)$ under the basis of $\left|\phi_1\right\rangle$ and $\left|\phi_2\right\rangle$ is diagonal,

$$\frac{1}{\hbar}(L_z + 2S_z) = \begin{pmatrix} m+\frac{1}{2} & 0 \\ 0 & m-\frac{1}{2} \end{pmatrix},$$

Thus the resultant matrix is given by

$$\hat{H}_1 = \frac{\xi\hbar^2}{4}\begin{pmatrix} (m-\frac{1}{2}) & \sqrt{(l+m+\frac{1}{2})(l-m+\frac{1}{2})} \\ \sqrt{(l+m+\frac{1}{2})(l-m+\frac{1}{2})} & -(m+\frac{1}{2}) \end{pmatrix}$$
$$+\mu_B B\begin{pmatrix} m+\frac{1}{2} & 0 \\ 0 & m-\frac{1}{2} \end{pmatrix}$$

We solve the eigenvalue problem. For simplicity we put

$$\frac{\xi\hbar^2}{4} = \frac{1}{2}\alpha, \qquad \beta = \mu_B B.$$

The matrix (2x2) is given by

$$\hat{H}_1 = \frac{\alpha}{2}\begin{pmatrix} m-\frac{1}{2} & \sqrt{(l+m+\frac{1}{2})(l-m+\frac{1}{2})} \\ \sqrt{(l+m+\frac{1}{2})(l-m+\frac{1}{2})} & -(m+\frac{1}{2}) \end{pmatrix} + \beta\begin{pmatrix} m+\frac{1}{2} & 0 \\ 0 & m-\frac{1}{2} \end{pmatrix};$$

or

$$\hat{H}_1 = \frac{\alpha}{2}\begin{pmatrix} m-\frac{1}{2} & k \\ k & -(m+\frac{1}{2}) \end{pmatrix} + \beta\begin{pmatrix} m+\frac{1}{2} & 0 \\ 0 & m-\frac{1}{2} \end{pmatrix},$$

where for simplicity we use

$$k = \sqrt{(l+m+\frac{1}{2})(l-m+\frac{1}{2})}\ .$$

We solve the eigenvalue problem of the matrix $\hat{H}_1$ (2 x 2 matrix). Thus the eigenvalues are

$$\lambda_1 = -\frac{\alpha}{4} + \beta m + \frac{1}{2}\sqrt{\alpha^2 (l+\frac{1}{2})^2 + 2\alpha\beta m + \beta^2)}\,,$$

$$\lambda_2 = -\frac{\alpha}{4} + \beta m - \frac{1}{2}\sqrt{\alpha^2 (l+\frac{1}{2})^2 + 2\alpha\beta m + \beta^2)}\,.$$

We introduce the ratio ζ as

$$\varsigma = \frac{\beta}{\alpha}.$$

Then we have

$$\lambda_1 = \frac{\alpha}{4}(-1 + 4\varsigma m + \frac{1}{2}\sqrt{(l+\frac{1}{2})^2 + 2\varsigma m + \varsigma^2)}\,,$$

and

$$\lambda_2 = \frac{\alpha}{4}(-1 + 4\varsigma m - \frac{1}{2}\sqrt{(l+\frac{1}{2})^2 + 2\varsigma m + \varsigma^2)}\,.$$

For $\varsigma << 1$ (weak field side)

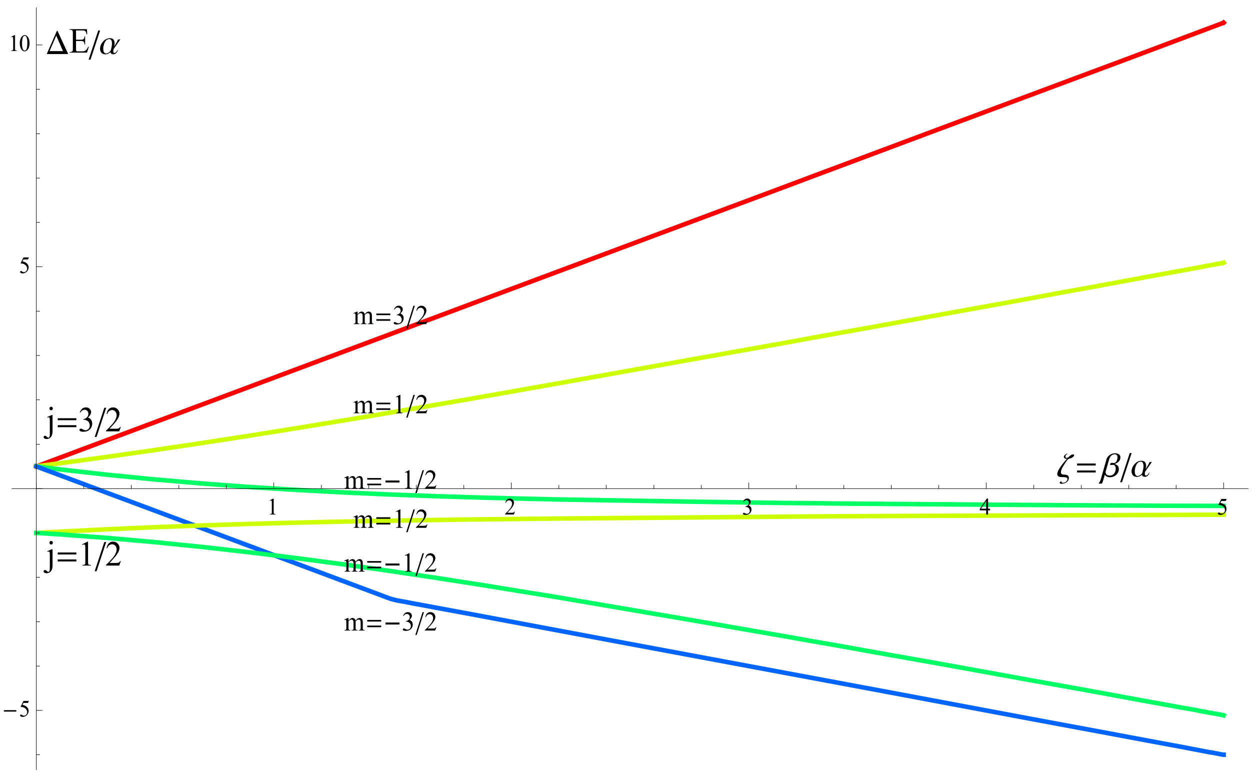
$$\lambda_1 = \frac{\alpha}{2} l + \beta m \frac{2l+2}{2l+1}\,,$$

$$\lambda_2 = -\frac{\alpha}{2}(l+1) + \beta m \frac{2l}{2l+1}\,.$$

The first term is from the spin-orbit interaction and the second term is from the Zeeman effect.

For $\varsigma >> 1$ (strong field side)

$$\lambda_1 = \alpha\varsigma(m+\frac{1}{2}) = \beta(m+\frac{1}{2}), \qquad \lambda_2 = \alpha\varsigma(m-\frac{1}{2}) = \beta(m-\frac{1}{2}).$$



((**Mathematica**))

```
Clear["Global`*"]; rule1 = {Sqrt[k^2 + m^2] → L + 1/2};
rule2 = {k → Sqrt[(L - m + 1/2) (L + m + 1/2)]};
A1 = α/2 {{m - 1/2, k}, {k, -(m + 1/2)}} + β {{m + 1/2, 0}, {0, (m - 1/2)}};
eq1 = Eigensystem[A1];
λ1 = eq1[[1, 2]] /. rule1 /. rule2 // Simplify[#, L > 0] &
```

$$\frac{1}{4}\left(-\alpha+4\,m\,\beta+\sqrt{(\alpha+2\,L\,\alpha)^2+8\,m\,\alpha\,\beta+4\,\beta^2}\right)$$

```
λ2 = eq1[[1, 1]] /. rule1 /. rule2 // Simplify[#, L > 0] &
```

$$-\frac{\alpha}{4}+m\,\beta-\frac{1}{4}\sqrt{(\alpha+2\,L\,\alpha)^2+8\,m\,\alpha\,\beta+4\,\beta^2}$$

```
λ11 = λ1 /. {β → ξ α} // Simplify[#, α > 0] &
```

$$\frac{1}{4}\,\alpha\left(-1+4\,m\,\xi+\sqrt{1+4\,L+4\,L^2+8\,m\,\xi+4\,\xi^2}\right)$$

```
λ22 = λ2 /. {β → ξ α} // Simplify[#, α > 0] &
```

$$-\frac{1}{4}\,\alpha\left(1-4\,m\,\xi+\sqrt{1+4\,L+4\,L^2+8\,m\,\xi+4\,\xi^2}\right)$$

```
Series[λ11, {ξ, 0, 2}] // Simplify[#, 2 L + 1 > 0] &
```

$$\frac{L\,\alpha}{2}+\frac{2\,(1+L)\,m\,\alpha\,\xi}{1+2\,L}+\frac{\left(1+4\,L+4\,L^2-4\,m^2\right)\alpha\,\xi^2}{2\,(1+2\,L)^3}+O[\xi]^3$$

```
Series[λ22, {ξ, 0, 2}] // Simplify[#, 2 L + 1 > 0] &
```

$$-\frac{1}{2}\,(1+L)\,\alpha+\frac{2\,L\,m\,\alpha\,\xi}{1+2\,L}-\frac{\left(\left(1+4\,L+4\,L^2-4\,m^2\right)\alpha\right)\xi^2}{2\,(1+2\,L)^3}+O[\xi]^3$$

((**Note**))

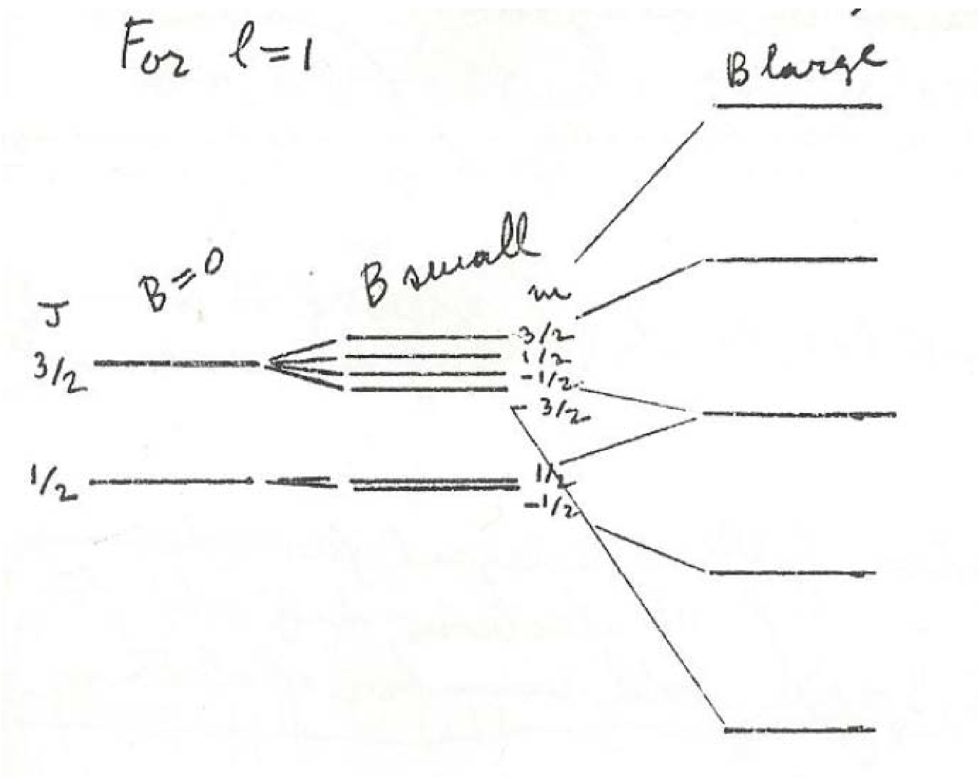


Fig. From the book of E. Fermi, Notes on Quantum Mechanaics (The University of Chicago, 1961)

6. Zeeman effect in the strong magnetic field (Paschen Back effect)

We consider the case where the magnetic field is strong enough that the Zeeman shifts are much larger than the fine-structure shifts. The perturbation assumption regarding the Zeeman effect is no longer valid. It is more appropriate to include the Zeeman Hamiltonian,

$$\hat{H} = \hat{H}_0 + \hat{H}_B = \hat{H}_0 - \hat{\boldsymbol{\mu}} \cdot \boldsymbol{B} = \hat{H}_0 + \frac{\mu_B}{\hbar}(\hat{\boldsymbol{L}} + 2\hat{\boldsymbol{S}}) \cdot \boldsymbol{B} ,$$

where

$$\hat{\boldsymbol{\mu}} = -\frac{\mu_B}{\hbar}(\hat{\boldsymbol{L}} + 2\hat{\boldsymbol{S}}) .$$

We note that

$$[\hat{H}_0,\hat{L}_x]=0\,,\quad [\hat{H}_0,\hat{L}_y]=0\,,\quad [\hat{H}_0,\hat{L}_z]=0\,,\quad [\hat{H}_0,\hat{\boldsymbol{L}}^2]=0$$

$$[\hat{H}_B,\hat{L}_z]=0\quad ,\qquad [\hat{H}_B,\hat{\boldsymbol{L}}^2]=0$$

$$[\hat{H}_0,\hat{S}_x]=0\,,\quad [\hat{H}_0,\hat{S}_y]=0\,,\quad [\hat{H}_0,\hat{S}_z]=0\,,\quad [\hat{H}_0,\hat{\boldsymbol{S}}^2]=0\,,$$

$$[\hat{H}_B,\hat{S}_z]=0\quad ,\qquad [\hat{H}_B,\hat{\boldsymbol{S}}^2]=0$$

Then we have

$$[\hat{H}_0,\hat{L}_z]=0\,,\quad [\hat{H}_0,\hat{\boldsymbol{L}}^2]=0\,,\quad [\hat{H}_0,\hat{S}_z]=0\,,\quad [\hat{H}_0,\hat{\boldsymbol{S}}^2]=0\,,$$

$$[\hat{\boldsymbol{L}}^2,\hat{L}_z]=0\,,\quad [\hat{\boldsymbol{S}}^2,\hat{S}_z]=0\,,\quad [\hat{H}_0,\hat{H}_B]=0$$

$$[\hat{H}_B,\hat{L}_z]=0\quad ,\ [\hat{H}_B,\hat{\boldsymbol{L}}^2]=0$$

$$[\hat{H}_B,\hat{S}_z]=0\quad ,\ [\hat{H}_B,\hat{\boldsymbol{S}}^2]=0$$

We choose a simultaneous eigenket of $\hat{H}_B$, $\hat{H}_0$, $\hat{\boldsymbol{L}}^2$, $\hat{\boldsymbol{S}}^2$, $\hat{L}_z$, and $\hat{S}_z$

$$|\psi\rangle=|nlm\rangle\otimes|sm_s\rangle=|nlm\rangle|sm_s\rangle$$

Here the Zeeman Hamiltonian

$$\hat{H}_B=\frac{\mu_B B}{\hbar}(\hat{L}_z+2\hat{S}_z)\,,$$

in zeroth-order and treat the fine structure as a perturbation. We note that

$$\hat{H}_0|n;lm_l;sm_s\rangle=E_n|n;lm_l;sm_s\rangle\,,$$

$$\hat{H}_B\left|n;lm_l;sm_s\right\rangle = \frac{\mu_B B}{\hbar}(\hat{L}_z + 2\hat{S}_z)\left|n;lm_l;sm_s\right\rangle = \mu_B B(m_l + 2m_s)\left|n;lm_l;sm_s\right\rangle .$$

The Zeeman energy is the expectation values,

$$E_{Zeeman}{}^{(1)} = \frac{\mu_B B}{\hbar}\left\langle n;lm_l;sm_s\right|(L_z + 2S_z)\left|n;lm_l;sm_s\right\rangle = \mu_B B(m_l + 2m_s)$$

We now treat the spin-orbit interaction as a perturbation to the zeroth order state that include the Zeeman interaction.

$$\begin{aligned}
E_{s0}{}^{(1)} &= \left\langle n;lm_l;sm_s\right|\hat{H}_{so}\left|n;lm_l;sm_s\right\rangle \\
&= \xi\left\langle n;lm_l;sm_s\right|\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}\left|n;lm_l;sm_s\right\rangle \\
&= \xi\left\langle n;lm_l;sm_s\right|\frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+) + \hat{L}_z\hat{S}_z\left|n;lm_l;sm_s\right\rangle \\
&= \xi\left\langle n;lm_l;sm_s\right|\hat{L}_z\hat{S}_z\left|n;lm_l;sm_s\right\rangle \\
&= \xi\hbar^2 m_l m_s \\
&= \frac{1}{2}m_e c^2\alpha^4\frac{m_l m_s}{n^3 l(l+\frac{1}{2})(l+1)}
\end{aligned}$$

where

$$\xi\hbar^2 = \frac{e^2\hbar^2}{2m_e{}^2c^2}\frac{1}{n^3 a_B{}^3 l(l+1/2)(l+1)} = \frac{1}{2}m_e c^2\alpha^4\frac{1}{n^3 l(l+1/2)(l+1)}$$

with

$$\alpha = \frac{e^2}{\hbar c}, \qquad a_B = \frac{\hbar^2}{me^2} .$$

Note that $E_{s0}{}^{(1)}$ is independent of the magnetic field. Thus we get

$$\Delta E^{(1)} = E_B{}^{(1)} + E_{so}{}^{(1)} = \mu_B B(m_l + 2m_s) + \frac{1}{2} m_e c^2 \alpha^4 \frac{m_l m_s}{n^3 l(l+\frac{1}{2})(l+1)}$$

or

$$\frac{\Delta E^{(1)}}{\mu_B B_0} = (m_l + 2m_s)\frac{B}{B_0} + \frac{1}{2}\frac{m_e c^2 \alpha^4}{\mu_B B_0}\frac{m_l m_s}{n^3 l(l+\frac{1}{2})(l+1)}$$

where B_0 is the characteristic magnetic field.

((**Example**))

The 2p state for the hydrogen. $n = 2$, $l = 1$, s = 1/2. $m_l = 1, 0, -1$. $m_s = 1/2, -1/2$. $x = \frac{B}{B_0}$.
$k = \frac{1}{2}\frac{m_e c^2 \alpha^4}{\mu_B B_0}$.

We make a plot of $\frac{\Delta E^{(1)}}{\mu_B B_0}$ as a function of $x = \frac{B}{B_0}$;

$$\frac{\Delta E^{(1)}}{\mu_B B_0} = (m_l + 2m_s)x + k\frac{m_l m_s}{n^3 l(l+\frac{1}{2})(l+1)}.$$

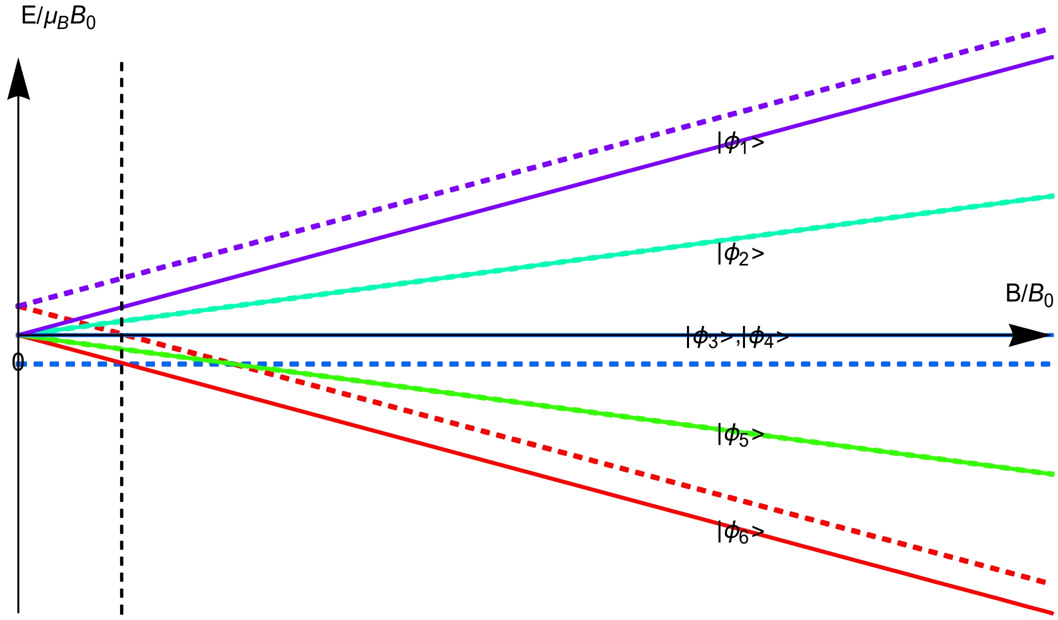


Fig. Strong-field Zeeman structure of the 2p states of hydrogen. Solid lines show the the Zeeman levels, while the dashed lines shows the addition of the Zeeman contribution and the spin-orbit interaction. The quantum numbers indicate the uncoupled basis states. The vertical dashed line denotes $x = \dfrac{B}{B_0} = 1$.

$|\phi_1\rangle = |m_l = 1, m_s = 1/2\rangle$, $\quad |\phi_2\rangle = |m_l = 0, m_s = 1/2\rangle$,

$|\phi_3\rangle = |m_l = 1, m_s = -1/2\rangle$, $\quad |\phi_4\rangle = |m_l = -1, m_s = 1/2\rangle$,

$|\phi_5\rangle = |m_l = 0, m_s = -1/2\rangle$, $\quad |\phi_6\rangle = |m_l = -1, m_s = -1/2\rangle$.

REFERENCES

D.H. McIntyre, *Quantum Mechanics A Paradigms Approach* (Pearson Education, 2012).

J.J. Sakurai and J. Napolitano, *Modern Quantum Mechanics*, 2nd edition (Addison-Wesley, 2011).

E. Fermi, *Notes on Quantum Mechanics* (The University of Chicago Press, 1961).

A. Landé, *Foundations of Quantum Theory A study in Continuity and Symmetry* (Yale University Press, 1955).

J. Binney and D. Skinner, *The Physics of Quantum Mechanics* (Oxford, 2014).

APPENDIX A. Landè g-factor

The magnetic moment is defined by

$$\hat{\boldsymbol{\mu}} = -\frac{\mu_B}{\hbar}(\hat{\boldsymbol{L}} + 2\hat{\boldsymbol{S}})$$

The total angular momentum is

$$\hat{\boldsymbol{J}} = \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}$$

The expectation value of the *m*-th component of the magnetic moment $\boldsymbol{\mu}$ can be obtained from the projection theorem (decomposition theorem of the second kind, see Rose),

In

$$\langle j,m|\hat{T}_q^{(1)}|j,m\rangle = \frac{< j \| \hat{\boldsymbol{J}}\cdot\hat{\boldsymbol{T}}^{(1)} \| j >}{\hbar^2 j(j+1)}\langle j,m|\hat{J}_q|j,m\rangle$$

we put

$$\hat{T}_q^{(1)} = \hat{\mu}_q, \qquad \hat{\boldsymbol{J}}\cdot\hat{\boldsymbol{T}}^{(1)} = \hat{\boldsymbol{J}}\cdot\hat{\boldsymbol{\mu}}$$

Then we get

$$\langle j,m|\hat{\mu}_q|j,m\rangle = \frac{< j \| \hat{\boldsymbol{J}}\cdot\hat{\boldsymbol{\mu}} \| j >}{\hbar^2 j(j+1)}\langle j,m|\hat{J}_q|j,m\rangle$$

Now we have

$$\hat{\boldsymbol{\mu}}\cdot\hat{\boldsymbol{J}} = -\frac{\mu_B}{\hbar}(\hat{\boldsymbol{L}} + 2\hat{\boldsymbol{S}})\cdot(\hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}) = -\frac{\mu_B}{\hbar}(\hat{\boldsymbol{L}}^2 + 2\hat{\boldsymbol{S}}^2 + 3\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}})\cdot$$

and

$$\hat{\boldsymbol{J}}^2 = \hat{\boldsymbol{L}}^2 + \hat{\boldsymbol{S}}^2 + 2\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}$$

or

$$\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}} = \frac{\hat{\boldsymbol{J}}^2 - \hat{\boldsymbol{L}}^2 - \hat{\boldsymbol{S}}^2}{2}$$

Then we get

$$\hat{\boldsymbol{\mu}} \cdot \hat{\boldsymbol{J}} = \hat{\boldsymbol{J}} \cdot \hat{\boldsymbol{\mu}} \cdot = -\frac{\mu_B}{\hbar}[\hat{\boldsymbol{L}}^2 + 2\hat{\boldsymbol{S}}^2 + \frac{3}{2}(\hat{\boldsymbol{J}}^2 - \hat{\boldsymbol{L}}^2 - \hat{\boldsymbol{S}}^2)] \cdot$$

and

$$< j \| \hat{\boldsymbol{J}} \cdot \hat{\boldsymbol{\mu}} \| j >= -\frac{\mu_B}{\hbar}\hbar^2 \{l(l+1) + 2s(s+1) + \frac{3}{2}[(j(j+1) - l(l+1) - s(s+1)]\}$$

Then the expectation value of the magnetic moment along the z axis is

$$\begin{aligned}
\langle j,m|\hat{\mu}_0| j,m\rangle &= \frac{< j \| \hat{\boldsymbol{J}} \cdot \hat{\boldsymbol{\mu}} \| j >}{\hbar^2 j(j+1)} \langle j,m|\hat{J}_0| j,m\rangle \\
&= -\frac{\mu_B}{\hbar}\frac{m\hbar}{\hbar^2 j(j+1)}\hbar^2 \{l(l+1) + 2s(s+1) \\
&\quad + \frac{3}{2}[(j(j+1) - l(l+1) - s(s+1)]\} \\
&= -\frac{m\mu_B}{2j(j+1)}[3(j(j+1) - l(l+1) + s(s+1)]
\end{aligned}$$

since $|j,m\rangle$ is a joint eigenstate of $\hat{\boldsymbol{J}}^2$, $\hat{\boldsymbol{L}}^2$, $\hat{\boldsymbol{S}}^2$, and $\hat{J}_0 = \hat{J}_z$ with eigenvalues $\hbar^2 j(j+1)$, $\hbar^2 l(l+1)$, $\hbar^2 s(s+1)$, and $\hbar m$, respectively.

Here we introduce the Landè g-factor as

$$\hat{\boldsymbol{\mu}} = -\frac{g_J \mu_B}{\hbar}\hat{\boldsymbol{J}}$$

Then we have

$$\langle j,m|\hat{\mu}_0| j,m\rangle = -\frac{g_J \mu_B}{\hbar}\langle j,m|\hat{J}_0| j,m\rangle = -\frac{g_J \mu_B}{\hbar} m\hbar = -mg_J \mu_B$$

and

$$g_J = \frac{3}{2} + \frac{s(s+1) - l(l+1)}{2j(j+1)}$$

APPENDIX-B. The expectation value of S_z

Since

$$\hat{\boldsymbol{S}} \cdot \hat{\boldsymbol{J}} \cdot = \hat{\boldsymbol{S}} \cdot (\hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}) = \hat{\boldsymbol{S}}^2 + \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}} = \hat{\boldsymbol{S}}^2 + \frac{\hat{\boldsymbol{J}}^2 - \hat{\boldsymbol{L}}^2 - \hat{\boldsymbol{S}}^2}{2} = \frac{\hat{\boldsymbol{J}}^2 - \hat{\boldsymbol{L}}^2 + \hat{\boldsymbol{S}}^2}{2}$$

we get the expectation of S_z as

$$\begin{aligned}
\langle j, m | \hat{S}_0 | j, m \rangle &= \frac{< j \| \hat{\boldsymbol{J}} \cdot \hat{\boldsymbol{S}} \| j >}{\hbar^2 j(j+1)} \langle j, m | \hat{J}_0 |; j, m \rangle \\
&= \frac{m\hbar}{2\hbar^2 j(j+1)} \hbar^2 [j(j+1) - l(l+1) + s(s+1)] \\
&= \frac{m\hbar}{2} [1 + \frac{s(s+1) - l(l+1)}{j(j+1)}]
\end{aligned}$$

where we use the projection theorem.