Spin-orbit interaction

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In quantum physics, the **spin–orbit interaction** is an interaction of a particle's spin with its motion. The first and best known example of this is that spin–orbit interaction causes shifts in an electron's atomic energy levels due to electromagnetic interaction between the electron's spin and the magnetic field generated by the electron's orbit around the nucleus.

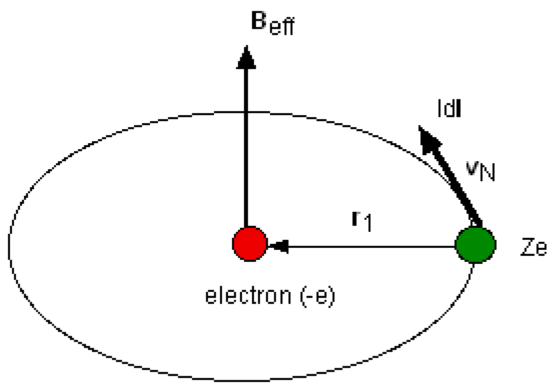
((Llewellyn Hilleth Thomas))

http://www.aip.org/history/acap/biographies/bio.jsp?thomasl

Llewellyn Hilleth Thomas (21 October 1903 – 20 April 1992) was a British physicist and applied mathematician. He is best known for his contributions to atomic physics, in particular: Thomas precession, a correction to the spin-orbit interaction in quantum mechanics, which takes into account the relativistic time dilation between the electron and the nucleus of an atom. The Thomas–Fermi model, a statistical model of the atom subsequently developed by Dirac and Weizsäcker, which later formed the basis of density functional theory. Thomas collapse - effect in few-body physics, which corresponds to infinite value of the three body binding energy for zero-range potentials.
http://en.wikipedia.org/wiki/Llewellyn_Thomas

1. Biot-Savart law

The electron has an orbital motion around the nucleus. This also implies that the nucleus has an orbital motion around the electron. The motion of nucleus produces an orbital current. From the Biot-Savart's law, it generates a magnetic field on the electron.



The current I due to the movement of nucleus (charge Ze, e>0) is given by

$$I d\boldsymbol{l} = Ze\boldsymbol{v}_N ,$$

where $\vec{v}_N$ is the velocity of the nucleus and $\frac{d\boldsymbol{l}}{dt} = \boldsymbol{v}_N$. Note that

$$I d\boldsymbol{l} = \frac{\Delta q}{\Delta t} d\boldsymbol{l} = \Delta q \frac{d\boldsymbol{l}}{dt} = Ze\boldsymbol{v}_N .$$

The effective magnetic field at the electron at the origin is

$$\boldsymbol{B}_{eff} = \frac{I}{c} \frac{d\boldsymbol{l} \times \boldsymbol{r}_1}{\left|\boldsymbol{r}_1\right|^3} , \qquad \boldsymbol{v}_N = v\boldsymbol{e}_\theta$$

where v is the velocity of the electron. Then we have

$$\boldsymbol{B}_{eff} = \frac{Ze}{c} \frac{\boldsymbol{v}_N \times \boldsymbol{r}_1}{\left|\boldsymbol{r}_1\right|^3} = \frac{Ze}{c} \frac{v\boldsymbol{e}_\theta \times \boldsymbol{r}_1}{\left|\boldsymbol{r}_1\right|^3} .$$

Since $\boldsymbol{r}_1 = -\boldsymbol{r}$, $\boldsymbol{B}_{eff}$ can be rewritten as

$$\vec{\boldsymbol{B}}_{eff} = -\frac{Ze}{c} \frac{v\boldsymbol{e}_\theta \times \boldsymbol{r}}{\left|\boldsymbol{r}\right|^3} = \frac{Zev}{c} \frac{\boldsymbol{r} \times \boldsymbol{e}_\theta}{\left|\boldsymbol{r}\right|^3} = \frac{Zev}{c} \frac{\boldsymbol{e}_z}{\left|\boldsymbol{r}\right|^2} = \frac{Zem_e v}{m_e c\left|\boldsymbol{r}\right|^2} \boldsymbol{e}_z$$

where m_e is the mass of electron. The Coulomb potential energy is given by

$$V_c(r) = -\frac{Ze^2}{r} , \qquad \frac{dV_c(r)}{dr} = \frac{Ze^2}{r^2} .$$

Thus we have

$$\boldsymbol{B}_{eff} = \frac{Ze^2 rv}{cer^3}\boldsymbol{e}_z = \frac{1}{m_e cer}\frac{Ze^2}{r^2}m_e rv\boldsymbol{e}_z = \frac{1}{m_e cer}\frac{dV_c(r)}{dr}L_z\boldsymbol{e}_z ,$$

or

$$\boldsymbol{B}_{eff} = \frac{1}{m_e ce}\frac{1}{r}\frac{dV_c(r)}{dr}L_z\boldsymbol{e}_z ,$$

where L_z is the *z*-component of the orbital angular momentum, $L_z = m_e vr$.

2. Derivation of the expression for the spin-orbit interaction

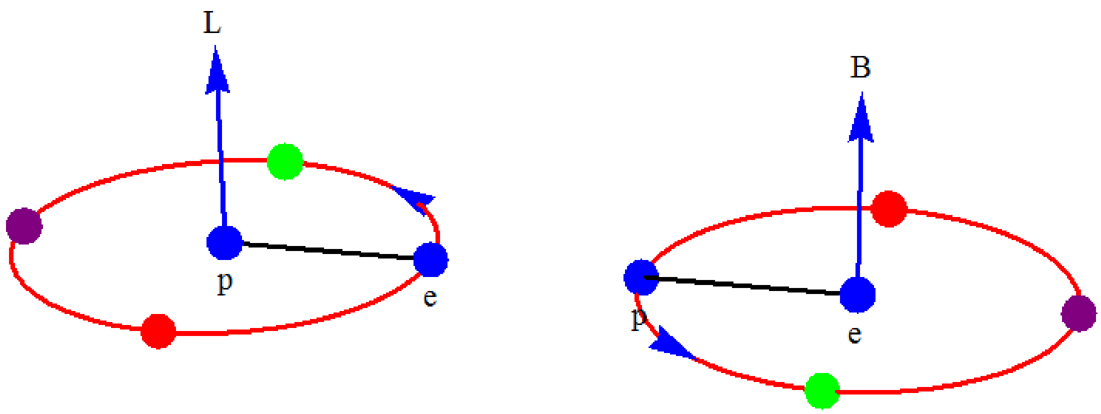


Fig. Electron in the proton frame, and proton in the electron frame. The direction of magnetic field ***B*** produced by the proton is the same as that of the orbital angular momentum ***L*** of the electron (the *z* axis in this figure).

We consider the circular motion of the nucleus (*e*) around an electron at the center. The nucleus rotates around the electron at the uniform velocity *v*. Note that the velocity of the proton in the electron frame is the same as the electron in the proton frame. The magnetic field (in cgs) at the center of the circle along with the current *I* flow.

$$B = \frac{2\pi I}{cr}.$$

according to the Biot-Savart law. The current *I* is given by

$$I = \frac{e}{T} = \frac{e}{\frac{2\pi r}{v}} = \frac{ev}{2\pi r},$$

where T is the period. Then the magnetic field $\boldsymbol{B}$ at the site of the electron (the proton frame) can be expressed as

$$\boldsymbol{B} = \frac{em_e v_N r}{m_e c r^3}\boldsymbol{e}_z = \frac{e\boldsymbol{L}}{m_e c r^3},$$

where $\boldsymbol{L}$ is the orbital angular momentum of the electron (the electron frame). Note that the direction of $\boldsymbol{B}$ is the same as that of $\boldsymbol{L}$. The spin magnetic moment is given by

$$\boldsymbol{\mu}_s = -\frac{2\mu_B}{\hbar}\boldsymbol{S},$$

where $\boldsymbol{S}$ is the spin angular momentum and μ_B is the Bohr magneton,

$$\mu_B = \frac{e\hbar}{2m_e c}.$$

Then the Zeeman energy of the electron is given by

$$H = -\frac{1}{2}\boldsymbol{\mu}_s \cdot \boldsymbol{B} = -\frac{1}{2}(-\frac{2\mu_B}{\hbar}\boldsymbol{S}) \cdot \left(\frac{e\boldsymbol{L}}{m_e c r^3}\right) = \frac{e^2}{2m_e^2 c^2 r^3}\boldsymbol{L}\cdot\boldsymbol{S},$$

where the factor (1/2) is the Thomas correction. In quantum mechanics we use the notation

$$\hat{H}_{so} = \frac{e^2}{2m_e^2 c^2}\left\langle \frac{1}{r^3} \right\rangle_{av} \hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}.$$

3. Thomas correction

The spin magnetic moment is defined by

$$\boldsymbol{\mu}_s = -\frac{2\mu_B}{\hbar}\boldsymbol{S},$$

where $\boldsymbol{S}$ is the spin angular momentum. Then the Zeeman energy is given by

$$\begin{aligned} H_{so} &= -\frac{1}{2}\boldsymbol{\mu}_s \cdot \boldsymbol{B}_{eff} = -\frac{1}{2}\left(-\frac{2\mu_B}{\hbar}\boldsymbol{S}\right)\cdot\left(\frac{1}{m_e c e}\frac{1}{r}\frac{dV_c(r)}{dr}\boldsymbol{L}\right) \\ &= \frac{1}{2m_e^2 c^2}\frac{1}{r}\frac{dV_c(r)}{dr}\boldsymbol{S}\cdot\boldsymbol{L} \\ &= \xi(\boldsymbol{S}\cdot\boldsymbol{L}) \end{aligned}$$

where the factor 1/2 is the Thomas correction and the Bohr magneton μ_B is given by

$$\mu_B = \frac{e\hbar}{2m_e c}.$$

Thomas factor 1/2, which represents an additional relativistic effect due to the acceleration of the electron. The electron spin, magnetic moment, and spin-orbit interaction can be derived directly from the Dirac relativistic electron theory. The Thomas factor is built in the expression.

$$H_{so} = \xi \boldsymbol{S} \cdot \boldsymbol{L},$$

with

$$\xi = \left\langle \frac{1}{2m_e^2 c^2} \frac{1}{r} \frac{dV_c(r)}{dr} \right\rangle = \frac{1}{2}\left(\frac{e}{m_e c}\right)^2 \left\langle \frac{1}{r^3} \right\rangle_{av}.$$

When we use the formula

$$\left\langle r^{-3} \right\rangle = \frac{1}{n^3 a_B^{\ 3} l(l+1/2)(l+1)},$$

the spin-orbit interaction constant ξ is described by

$$\xi = \frac{e^2}{2m_e^2 c^2 n^3 a_B^{\ 3} l(l+1/2)(l+1)} = \frac{m_e e^8}{2c^2 n^3 \hbar^6 l(l+1/2)(l+1)}$$

where

$$a_B = \frac{\hbar^2}{m_e e^2} = 0.53 \text{ Å} \qquad \text{(Bohr radius).}$$

The energy level (negative) is given by

$$\left|E_n\right| = \frac{e^2}{2n^2 a_B} = \frac{\Re_0}{n^2},$$

where

$$\Re_0 = \frac{m_e e^4}{2\hbar^2} = \frac{e^2}{2a_B}.$$

The ratio $\hbar^2\xi/|E_n|$ is

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

with

$$\alpha = \frac{e^2}{\hbar c} = \frac{1}{137.037}$$

((**Note**)) For $l = 0$ the spin-orbit interaction vanishes and therefore $\xi = 0$ in this case.

((**Summary**))
The spin-orbit interaction serves to remove the l degeneracy of the eigenenergies of hydrogen atom. If the spin-orbit interaction is neglected, energies are dependent only on n (principal quantum number). In the presence of spin-orbit interaction (n, l, s = 1/2; j, m) are good quantum numbers. Energies are dependent only on (n, l, j).

4. Commutation relations

We introduce a new Hamiltonian given by

$$\hat{H} = \hat{H}_0 + \hat{H}_{so},$$

The total angular momentum $\boldsymbol{J}$ is the addition of the orbital angular momentum and the spin angular momentum,

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

The spin-orbit interaction is defined by

$$\hat{H}_{so} = \xi\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}} = \xi\frac{1}{2}(\hat{\boldsymbol{J}}^2 - \hat{\boldsymbol{L}}^2 - \hat{\boldsymbol{S}}^2).$$

where

$$\hat{\boldsymbol{L}}\times\hat{\boldsymbol{L}} = i\hbar\hat{\boldsymbol{L}}, \qquad \hat{\boldsymbol{S}}\times\hat{\boldsymbol{S}} = i\hbar\hat{\boldsymbol{S}},$$

and

$$[\hat{L}_x, \hat{S}_x] = 0, \quad [\hat{L}_x, \hat{S}_y] = 0, \quad [\hat{L}_x, \hat{S}_z] = 0,$$

$$[\hat{L}_y, \hat{S}_x] = 0, \quad [\hat{L}_y, \hat{S}_y] = 0, \quad [\hat{L}_y, \hat{S}_z] = 0,$$

$$[\hat{L}_z, \hat{S}_x] = 0, \quad [\hat{L}_z, \hat{S}_y] = 0, \quad [\hat{L}_z, \hat{S}_z] = 0.$$

$$[\hat{\boldsymbol{L}}^2, \hat{\boldsymbol{S}}^2] = 0$$

(a) The unperturbed Hamiltonian $\hat{H}_0$

The unperturbed Hamiltonian $\hat{H}_0$ commutes with all the components of $\hat{\boldsymbol{L}}$ and $\hat{\boldsymbol{S}}$.

(i)

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

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

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

(ii)

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

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

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

and

$$[\hat{H}_0, \hat{J}_z] = [\hat{H}_0, \hat{L}_z + \hat{S}_z] = 0.$$

We note that

$$[\hat{H}_0, \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}] = [\hat{H}_0, (\hat{L}_x \hat{S}_x + \hat{L}_y \hat{S}_y + \hat{L}_z \hat{S}_z)] = 0.$$

Then we have

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

or

$$[\hat{H}_0, \hat{\boldsymbol{J}}^2] = 0.$$

We also note that

$$[\hat{\boldsymbol{J}}^2, \hat{\boldsymbol{L}}^2] = [\hat{\boldsymbol{L}}^2 + \hat{\boldsymbol{S}}^2 + 2\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}, \hat{\boldsymbol{L}}^2] = 2[\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}, \hat{\boldsymbol{L}}^2] = 0,$$

$$[\hat{\boldsymbol{J}}^2, \hat{\boldsymbol{S}}^2] = [\hat{\boldsymbol{L}}^2 + \hat{\boldsymbol{S}}^2 + 2\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}, \hat{\boldsymbol{S}}^2] = 2[\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}, \hat{\boldsymbol{S}}^2] = 0,$$

$$\begin{aligned}[\hat{\boldsymbol{J}}^2, \hat{J}_z] &= [\hat{\boldsymbol{L}}^2 + \hat{\boldsymbol{S}}^2 + 2\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}, \hat{L}_z + \hat{S}_z] \\ &= 2[\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}, \hat{L}_z + \hat{S}_z] = 0 \\ &= -2[\hat{L}_z, \hat{L}_x]\hat{S}_x + 2[\hat{L}_y, \hat{L}_z]\hat{S}_y - 2\hat{L}_x[\hat{S}_z, \hat{S}_x] + 2\hat{L}_y[\hat{S}_y, \hat{S}_z] \\ &= -2i\hbar\hat{L}_y\hat{S}_x + 2i\hbar\hat{L}_x\hat{S}_y - 2i\hbar\hat{L}_x\hat{S}_y + 2i\hbar\hat{L}_y\hat{S}_x \\ &= 0\end{aligned}$$

$$[\hat{\boldsymbol{L}}^2, \hat{J}_z] = [\hat{\boldsymbol{L}}^2, \hat{L}_z + \hat{S}_z] = 0$$

$$[\hat{\boldsymbol{S}}^2, \hat{J}_z] = [\hat{\boldsymbol{S}}^2, \hat{L}_z + \hat{S}_z] = 0$$

Thus we conclude that $|\psi_0\rangle$ is the simultaneous eigenket of the mutually commuting observables $\{\hat{H}_0, \hat{\boldsymbol{L}}^2, \hat{\boldsymbol{S}}^2, \hat{\boldsymbol{J}}^2$, and $\hat{J}_z\}$.

$$|\psi_0\rangle = |n, l, s; j, m\rangle,$$

$$\hat{H}_0|\psi_0\rangle = E_n^{(0)}|\psi_0\rangle,$$

$$\hat{\boldsymbol{L}}^2|\psi_0\rangle = \hbar^2 l(l+1)|\psi_0\rangle,$$

$$\hat{\boldsymbol{S}}^2|\psi_0\rangle = \hbar^2 s(s+1)|\psi_0\rangle,$$

$$\hat{\boldsymbol{J}}^2|\psi_0\rangle = \hbar^2 j(j+1)|\psi_0\rangle,$$

$$\hat{J}_z|\psi_0\rangle = \hbar m|\psi_0\rangle.$$

(b) The perturbed Hamiltonian $\hat{H}_{so}$

Here we note that $\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}$ does not commute with $\hat{L}_z$ or $\hat{S}_z$.

$$\begin{aligned}[\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}, \hat{L}_z] &= -[\hat{L}_z, \hat{L}_x]\hat{S}_x + [\hat{L}_y, \hat{L}_z]\hat{S}_y \\ &= -i\hbar\hat{L}_y\hat{S}_x + i\hbar\hat{L}_x\hat{S}_y\end{aligned}$$

$$[\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{S}_z] = -\hat{L}_x[\hat{S}_z,\hat{S}_x] + \hat{L}_y[\hat{S}_y,\hat{S}_z]$$
$$= -i\hbar\hat{L}_x\hat{S}_y + i\hbar\hat{L}_y\hat{S}_x$$

These relations lead to the commutation relation

$$[\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{J}_z] = 0$$

These commutation relations can be also derived from the invariant of the scalar product $\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}$, under the rotation. The rotation operator around the z axis is given by $\hat{R}_z(\delta\theta) = \hat{1} - \frac{i}{\hbar}\hat{J}_z\delta\theta$. So we have

$[\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{J}_x] = 0$ from the rotation around the x axis.

$[\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{J}_y] = 0$ from the rotation around the y axis.

$[\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{J}_z] = 0$ from the rotation around the z axis.

Similarly we have

$$[\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{J}_x{}^2] = 0, \qquad [\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{J}_y{}^2] = 0, \qquad [\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{J}_z{}^2] = 0,$$

and

$$[\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{\boldsymbol{J}}^2] = 0$$

In summary, we have

$$[\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{\boldsymbol{J}}^2] = 0, \qquad [\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{J}_z] = 0, \qquad [\hat{\boldsymbol{J}}^2,\hat{J}_z] = 0.$$

Thus the state vector $|\psi\rangle$ is the simultaneous eigenkets of $\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}$, $\hat{\boldsymbol{J}}^2$, and $\hat{J}_z$. In other words,

$$\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}|\psi\rangle = \lambda|\psi\rangle,$$

$$\hat{\boldsymbol{J}}^2|\psi\rangle = \hbar^2 j(j+1)|\psi\rangle,$$

$$\hat{J}_z|\psi\rangle = \hbar m|\psi\rangle.$$

((**Note**))
E. Fermi, Notes on Quantum Mechanics, 2nd edition (University of Chicago, 1962)

$$[\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{L}_z]\neq 0\,, \qquad [\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{S}_z]\neq 0\,. \qquad [\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{J}_z]=0$$

Thus $\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}$ mixes states of same j, m and different m_l and m_s.

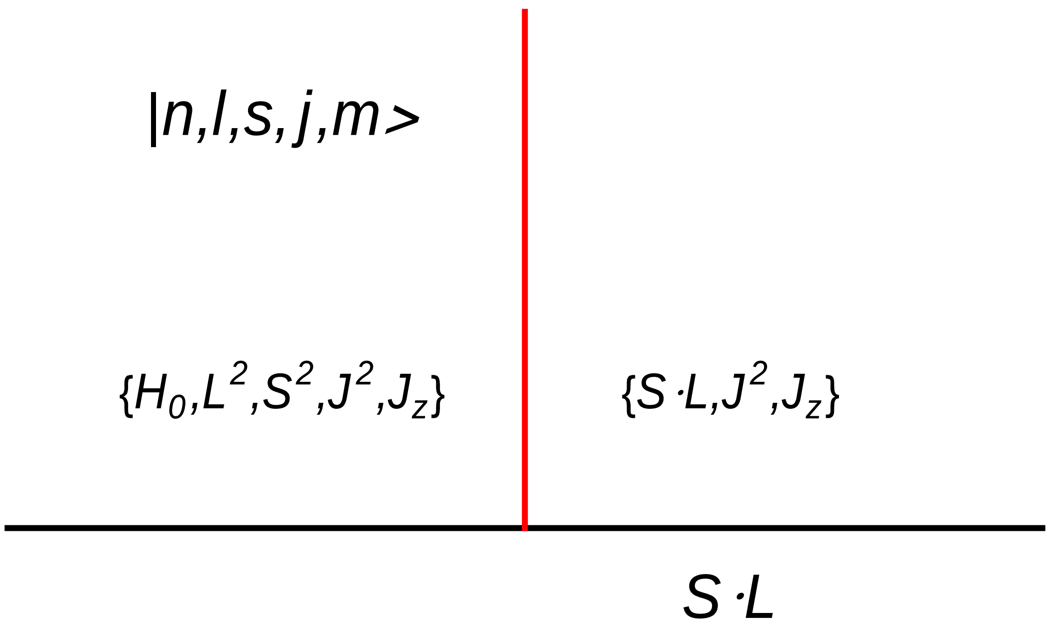


Fig. Perturbation due to the spin-orbit interaction. $|n,l,s,j,m\rangle$ is the simultaneous eigenkets of $\hat{H}_0$, $\hat{\boldsymbol{L}}^2$, $\hat{\boldsymbol{S}}^2$, $\hat{\boldsymbol{J}}^2$, and $\hat{J}_z$ without spin-orbit interaction. When the spin-orbit interaction is switched on, $\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}$ mixes states of same j, m and different m_l and m_s. $[\hat{H},\hat{\boldsymbol{J}}^2]=0$. $[\hat{H},\hat{J}_z]=0$. $\hat{H}$ is the total Hamiltonian. Note that $[\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{H}_0,]=0$, $[\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{\boldsymbol{J}}^2]=0$, $[\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{J}_z]=0$, $[\hat{\boldsymbol{J}}^2,\hat{J}_z]=0$. $[\hat{H}_0,\hat{\boldsymbol{J}}^2]=0$. $[\hat{H}_0,\hat{J}_z]=0$. $[\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{L}_z]\neq 0$, $[\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},\hat{S}_z]\neq 0$.

5. Application of the perturbation theory (degenerate case))

We need to choose the unperturbed states that diagonalize the perturbation **(Cardinal rule).** So the best way we can do is to choose the state

$$|\psi\rangle = |\,j,m\rangle\,,$$

where j and m are the good quantum numbers. The perturbation $\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}$ mixes states of same J_z and $\boldsymbol{J}^2$ but different L_z and S_z. Here we use the following notation.

$$\boldsymbol{J}^2 = \hbar^2 j(j+1), \qquad J_z = \hbar m, \qquad L_z = \hbar m_l, \qquad S_z = \hbar m_s;$$

with

$$m = m_l + m_s$$

where

$$m_l = l, l - 1, l - 2, \ldots, -l$$

$$m_s = 1/2, -1/2.$$

We note that the spin-orbit interaction occurs only for $l \geq 1$. In order to get the eigenvalues and eigenkets of $\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}$, we choose two states:

$$|\phi_1\rangle = \left| l, m_l = m - \frac{1}{2} \right\rangle \otimes \left| S = \frac{1}{2}, m_s = \frac{1}{2} \right\rangle,$$

$$|\phi_2\rangle = \left| l, m_l = m + \frac{1}{2} \right\rangle \otimes \left| S = \frac{1}{2}, m_s = -\frac{1}{2} \right\rangle$$

where $m = m_l + m_s$. Next we calculate the matrix element of $\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}$ under the basis of the kets, $|\phi_1\rangle$ and $|\phi_2\rangle$;

$$\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}} |\phi_1\rangle, \qquad \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}} |\phi_2\rangle.$$

or

$$\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}} = \begin{pmatrix} \langle \phi_1 | \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}} | \phi_1 \rangle & \langle \phi_1 | \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}} | \phi_2 \rangle \\ \langle \phi_2 | \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}} | \phi_1 \rangle & \langle \phi_2 | \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}} | \phi_2 \rangle \end{pmatrix}$$

We can solve the eigenvalue problem of this matrix (2x2), leading to the two eigenvalues. The corresponding eigenstates are denoted by

$$|\psi_1\rangle = \left| j = l + \frac{1}{2}, m \right\rangle, \qquad \text{for } j = l + \frac{1}{2}$$

$$|\psi_2\rangle = \left| j = l - \frac{1}{2}, m \right\rangle, \qquad \text{for } j = l - \frac{1}{2}$$

We will check the value of $j = l \pm \frac{1}{2}$ later. In fact the value of j can be obtained the triangular law as

$$D_l \times D_{s=1/2} = D_{l+1/2} + D_{l-1/2}$$

leading to

$$j = l + \frac{1}{2}, \qquad \text{and} \qquad j = l - \frac{1}{2}$$

Then the energy eigenvalues are obtained as

$$\begin{aligned}
\hat{H}_{so}\left| j = l + \frac{1}{2}, m \right\rangle &= \xi \frac{1}{2}(\hat{\boldsymbol{J}}^2 - \hat{\boldsymbol{L}}^2 - \hat{\boldsymbol{S}}^2)\left| j = l + \frac{1}{2}, m \right\rangle \\
&= \xi \frac{\hbar^2}{2}[j(j+1) - l(l+1) - \frac{3}{4})]\left| j = l + \frac{1}{2}, m \right\rangle \\
&= \xi \frac{\hbar^2}{2}[(l + \frac{1}{2})(l + \frac{3}{2}) - l(l+1) - \frac{3}{4})]\left| j = l + \frac{1}{2}, m \right\rangle \\
&= \frac{l\hbar^2}{2}\xi[\left| j = l + \frac{1}{2}, m \right\rangle
\end{aligned}$$

$$\begin{aligned}
\hat{H}_{so}\left| j = l - \frac{1}{2}, m \right\rangle &= \xi \frac{1}{2}(\hat{\boldsymbol{J}}^2 - \hat{\boldsymbol{L}}^2 - \hat{\boldsymbol{S}}^2)\left| j = l - \frac{1}{2}, m \right\rangle \\
&= \xi \frac{\hbar^2}{2}[j(j+1) - l(l+1) - \frac{3}{4})]\left| j = l - \frac{1}{2}, m \right\rangle \\
&= \xi \frac{\hbar^2}{2}[(l - \frac{1}{2})(l + \frac{1}{2}) - l(l+1) - \frac{3}{4})]\left| j = l - \frac{1}{2}, m \right\rangle \\
&= -\frac{(l+1)\hbar^2}{2}\xi[\left| j = l - \frac{1}{2}, m \right\rangle
\end{aligned}$$

In summary

(i) $\left| j = l + \frac{1}{2}, m \right\rangle$ is the eigenstate of $\hat{H}_{so}$ with the energy $\frac{l\xi\hbar^2}{2}$.

(ii) $\left| j = l - \frac{1}{2}, m \right\rangle$ is the eigenstate of $\hat{H}_{so}$ with the energy $-\frac{(l+1)\xi\hbar^2}{2}$.

6. The choice of $|\phi_1\rangle$ and $|\phi_2\rangle$ with the same *j* and *m*

6.1 *l* = 1, *s*=1/2, leading to *j* = 3/2 and *j* = ½

(a) $j = 1/2$ (m = 1/2 and m = 1/2)

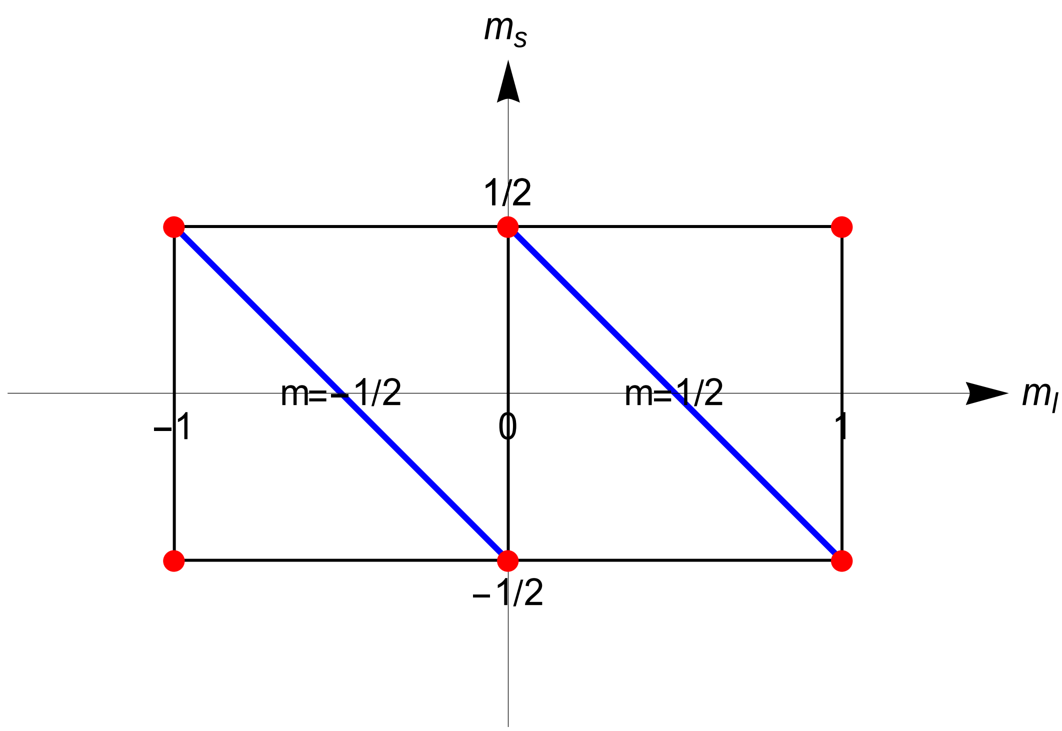


Fig. (m_l, m_s) plane for j = 1/2. l = 1 and s = 1/2. $m = m_l + m_s$ (denoted by blue lines).

For m = 1/2, the superposition of $\left|m_l = 0, m_3 = 1/2\right\rangle$ and $\left|m_l = 1, m_3 = -1/2\right\rangle$

For m = -1/2, the superposition of $\left|m_l = -1, m_3 = 1/2\right\rangle$ and $\left|m_l = 0, m_3 = 1/2\right\rangle$

(b) $j = 3/2$ (m = 3/2, 1/2, -1/2, and -3/2)

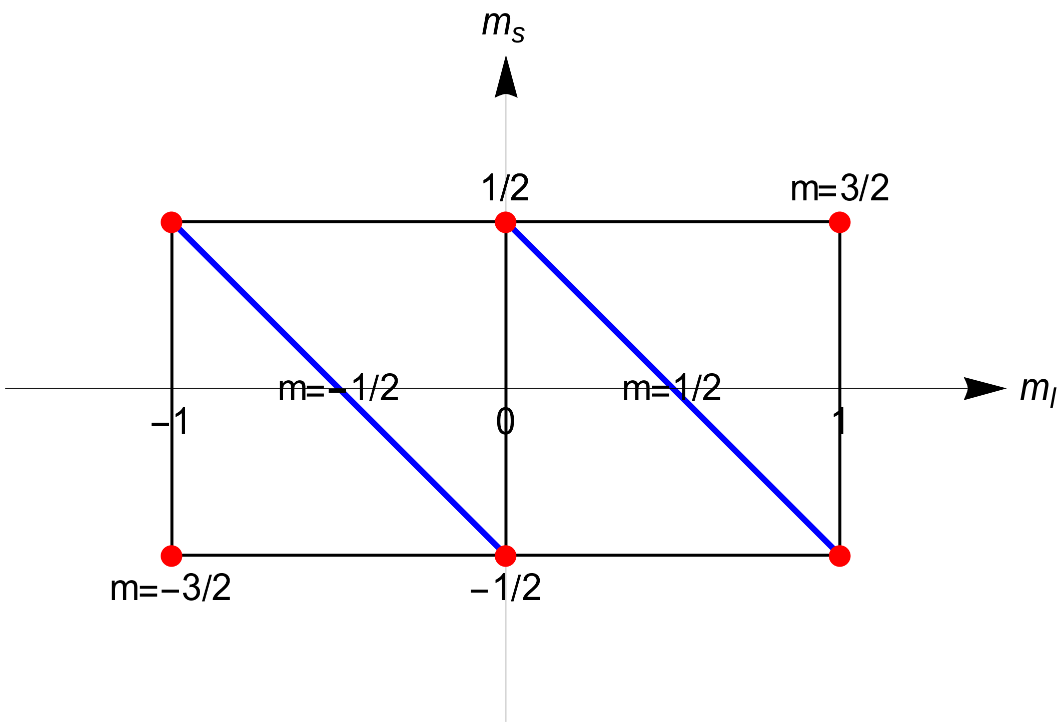


Fig. (m_l, m_s) plane for j = 3/2. l = 1 and s = 1/2. $m = m_l + m_s$ (denoted by blue lines).

For m = 3/2, the superposition of $|m_l = 1, m_3 = 1/2\rangle$

For m = 1/2, the superposition of $|m_l = 0, m_3 = 1/2\rangle$ and $|m_l = 1, m_3 = -1/2\rangle$

For m = -1/2, the superposition of $|m_l = -1, m_3 = 1/2\rangle$ and $|m_l = 0, m_3 = 1/2\rangle$

For m = -3/2, the superposition of $|m_l = -1, m_3 = -1/2\rangle$

6.2 l = 2, s=1/2, leading to j = 5/2 and j = 3/2

(a) j = 5/2 (m = 5/2, 3/2, 1/2, -1/2, -3/2, -5/2)

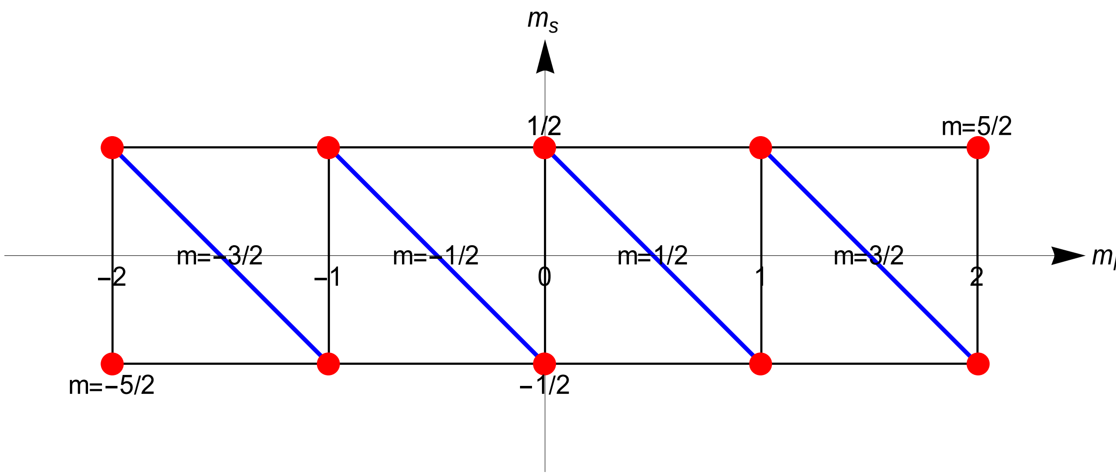


Fig. (m_l, m_s) plane for j = 5/2. l = 2 and s = 1/2. $m = m_l + m_s$ (denoted by blue lines).

For m = 5/2, the superposition of $|m_l = 2, m_3 = 1/2\rangle$

For m = 3/2, the superposition of $|m_l = 1, m_3 = 1/2\rangle$ and $|m_l = 2, m_3 = -1/2\rangle$

For m = 1/2, the superposition of $|m_l = 0, m_3 = 1/2\rangle$ and $|m_l = 1, m_3 = -1/2\rangle$

For m = -1/2, the superposition of $|m_l = -1, m_3 = 1/2\rangle$ and $|m_l = 0, m_3 = 1/2\rangle$

For m = -3/2, the superposition of $|m_l = -1, m_3 = -1/2\rangle$ and $|m_l = -2, m_3 = 1/2\rangle$

For m = 5/2, the superposition of $|m_l = 2, m_3 = 1/2\rangle$

(b) j = 3/2, (m = 3/2, 1/2, -1/2, -3/2)

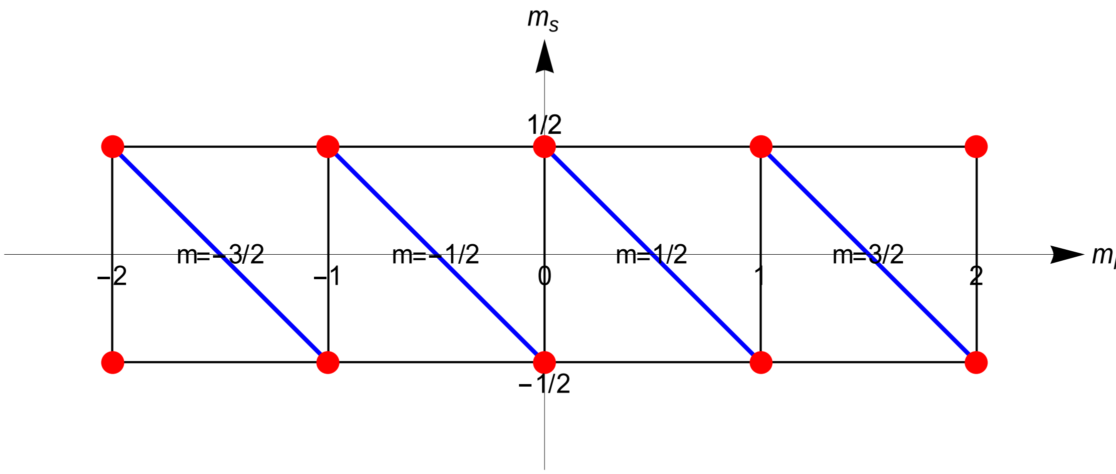


Fig. (m_l, m_s) plane for j = 3/2. l = 2 and s = 1/2. $m = m_l + m_s$ (denoted by blue lines).

For m = 3/2, the superposition of $|m_l = 1, m_3 = 1/2\rangle$ and $|m_l = 2, m_3 = -1/2\rangle$

For m = 1/2, the superposition of $|m_l = 0, m_3 = 1/2\rangle$ and $|m_l = 1, m_3 = -1/2\rangle$

For m = -1/2, the superposition of $|m_l = -1, m_3 = 1/2\rangle$ and $|m_l = 0, m_3 = 1/2\rangle$

For m = -3/2, the superposition of $|m_l = -1, m_3 = -1/2\rangle$ and $|m_l = -2, m_3 = 1/2\rangle$

6. Solving the eigenvalue problem

We calculate the matrix element of the spin-orbit interaction under the basis of

$$|\phi_1\rangle = \left|m_l = m - \frac{1}{2}, m_s = \frac{1}{2}\right\rangle = \left|l, m_l = m - \frac{1}{2}\right\rangle \otimes \left|S = \frac{1}{2}, m_s = \frac{1}{2}\right\rangle,$$

$$|\phi_2\rangle = \left|m_l = m + \frac{1}{2}, m_s = -\frac{1}{2}\right\rangle = \left|l, m_l = m + \frac{1}{2}\right\rangle \otimes \left|S = \frac{1}{2}, m_s = -\frac{1}{2}\right\rangle,$$

where m is fixed. Here we use the formula

$$\hat{J}_-|j,m\rangle = \hbar\sqrt{(j+m)(j-m+1)}|j,m-1\rangle,$$

$$\hat{J}_+|j,m\rangle = \hbar\sqrt{(j-m)(j+m+1)}|j,m+1\rangle,$$

$$\hat{S}_+|-\rangle = \hbar|+\rangle,$$

$$\hat{S}_{-}\left|+\right\rangle = \hbar\left|-\right\rangle,$$

$$\hat{\boldsymbol{J}}^2\left| j,m\right\rangle = \hbar^2 j(j+1)(\left| j,m\right\rangle,$$

where

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

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

$$\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}} = \hat{L}_z\cdot\hat{S}_z + \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+).$$

Then we get

$$\begin{aligned}
\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}\left|\phi_1\right\rangle &= \hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}\left|m_l = m-\frac{1}{2}, m_s = \frac{1}{2}\right\rangle \\
&= [\hat{L}_z\cdot\hat{S}_z + \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+)]\left|m_l = m-\frac{1}{2}, m_s = \frac{1}{2}\right\rangle \\
&= [\frac{\hbar^2}{2}(m-\frac{1}{2}) + \frac{1}{2}\hat{L}_+\hat{S}_-]\left|m_l = m-\frac{1}{2}, m_s = \frac{1}{2}\right\rangle \\
&= \frac{\hbar^2}{2}(m-\frac{1}{2})\left|m_l = m-\frac{1}{2}, m_s = \frac{1}{2}\right\rangle \\
&\quad + \frac{\hbar^2}{2}\sqrt{(l+m+\frac{1}{2})(l-m+\frac{1}{2})}\left|m_l = m+\frac{1}{2}, m_s = -\frac{1}{2}\right\rangle \\
&= \frac{\hbar^2}{2}[(m-\frac{1}{2})\left|\phi_1\right\rangle + \sqrt{(l+m+\frac{1}{2})(l-m+\frac{1}{2})}\left|\phi_2\right\rangle]
\end{aligned}$$

$$
\begin{aligned}
\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}|\phi_2\rangle &= \hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}\left|m_l = m+\frac{1}{2}, m_s = -\frac{1}{2}\right\rangle \\
&= [\hat{L}_z\cdot\hat{S}_z + \frac{1}{2}(\hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+)]\left|m_l = m+\frac{1}{2}, m_s = -\frac{1}{2}\right\rangle \\
&= [-\frac{\hbar^2}{2}(m+\frac{1}{2}) + \hat{L}_-\hat{S}_+]\left|m_l = m+\frac{1}{2}, m_s = -\frac{1}{2}\right\rangle \\
&= \frac{\hbar^2}{2}\sqrt{(l+m+\frac{1}{2})(l-m+\frac{1}{2})}\left|m_l = m-\frac{1}{2}, m_s = \frac{1}{2}\right\rangle \\
&\quad -\frac{\hbar^2}{2}(m+\frac{1}{2})\left|m_l = m+\frac{1}{2}, m_s = -\frac{1}{2}\right\rangle \\
&= \frac{\hbar^2}{2}[\sqrt{(l+m+\frac{1}{2})(l-m+\frac{1}{2})}|\phi_1\rangle - (m+\frac{1}{2})|\phi_2\rangle]
\end{aligned}
$$

Thus we obtain the matrix of $\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}$ under the basis of $|\phi_1\rangle$ and $|\phi_2\rangle$, 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 solve the eigenvalue problem. The eigenvalues are obtained as

$$\lambda_1 = l,\ \lambda_2 = -(l+1).$$

For $\lambda_1 = l$, the eigenket is obtained as

$$
\begin{aligned}
|\psi_1\rangle &= \sqrt{\frac{l+m+1/2}{2l+1}}|m_l = m-1/2, m_s = 1/2\rangle \\
&\quad + \sqrt{\frac{l-m+1/2}{2l+1}}|m_l = m+1/2, m_s = -1/2\rangle
\end{aligned}
$$

Using $\lambda_1 = l$, we get

$$\begin{aligned}\boldsymbol{J}^2 &= \hbar^2 j(j+1) \\ &= \boldsymbol{L}^2 + \boldsymbol{S}^2 + 2\boldsymbol{L}\cdot\boldsymbol{S} \\ &= \hbar^2[l(l+1) + \frac{3}{4} + \lambda_1]. \\ &= \hbar^2[l(l+1) + \frac{3}{4} + l] \\ &= \hbar^2(l+\frac{1}{2})(l+\frac{3}{2})\end{aligned}$$

which means that $j = l + \frac{1}{2}$

For $\lambda_2 = -(l+1)$, we have

$$\begin{aligned}|\psi_2\rangle = &-\sqrt{\frac{l-m+1/2}{2l+1}}|m_l = m-1/2, m_s = 1/2\rangle \\ &+\sqrt{\frac{l+m+1/2}{2l+1}}|m_l = m+1/2, m_s = -1/2\rangle\end{aligned}$$

Using $\lambda_2 = -(l+1)$, we get

$$\begin{aligned}\boldsymbol{J}^2 &= \hbar^2 j(j+1) \\ &= \boldsymbol{L}^2 + \boldsymbol{S}^2 + 2\boldsymbol{L}\cdot\boldsymbol{S} \\ &= \hbar^2[l(l+1) + \frac{3}{4} + \lambda_2] \\ &= \hbar^2[l(l+1) + \frac{3}{4} - (l+1)] = \hbar^2(l-\frac{1}{2})(l-\frac{1}{2}+1)\end{aligned}$$

which means that $j = l - \frac{1}{2}$.

Then we can obtain

(i) $\quad j = l + \frac{1}{2}$

$$|\psi_1\rangle = \left| j = l + \frac{1}{2}, m \right\rangle$$
$$= \sqrt{\frac{l+m+1/2}{2l+1}} |m_l = m - 1/2, m_s = 1/2\rangle$$
$$+ \sqrt{\frac{l-m+1/2}{2l+1}} |m_l = m + 1/2, m_s = -1/2\rangle$$

$$\hat{H}_{so}|\psi_1\rangle = \xi \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}} |\psi_1\rangle = \frac{l\xi\hbar^2}{2}|\psi_1\rangle$$ (which is independent of m)

(ii) $j = l - \frac{1}{2}$

$$|\psi_2\rangle = \left| j = l - \frac{1}{2}, m \right\rangle$$
$$= -\sqrt{\frac{l-m+1/2}{2l+1}} |m_l = m - 1/2, m_s = 1/2\rangle$$
$$+ \sqrt{\frac{l+m+1/2}{2l+1}} |m_l = m + 1/2, m_s = -1/2\rangle$$

$$\hat{H}_{so}|\psi_2\rangle = \xi \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}} |\psi_2\rangle = -\frac{(l+1)\xi\hbar^2}{2}|\psi_2\rangle$$ (which is independent of m).

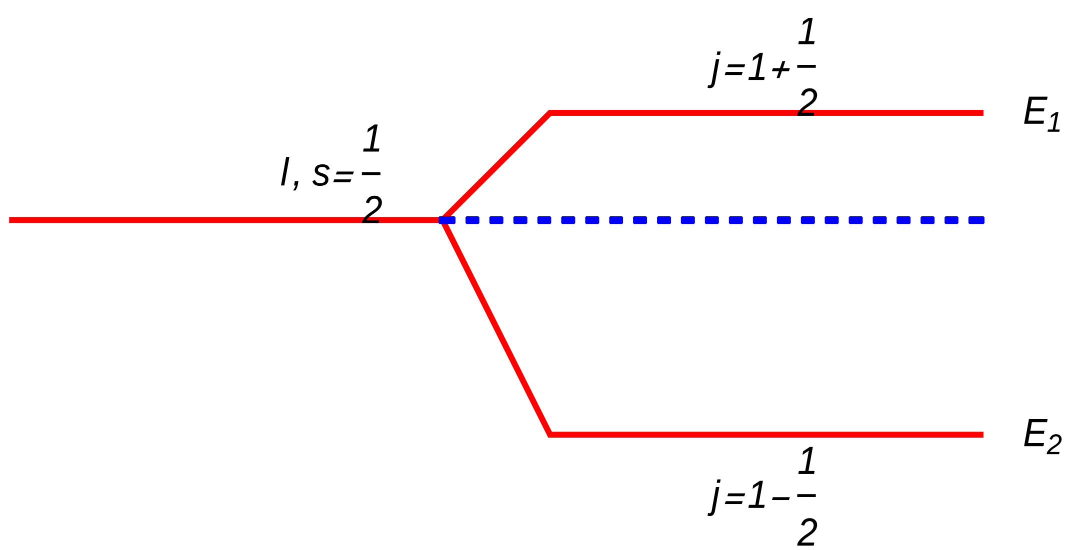


Fig. Splitting of the energy level due to the spin-orbit interaction. $E_1 = \frac{l\xi\hbar^2}{2}$. $E_2 = -\frac{(l+1)\xi\hbar^2}{2}$. This splitting is independent of the quantum number *m*.

7. Mathematica: the eigenvalue problem

```
Clear["Global`*"]; rule1 = {√(k² + m²) → L + 1/2};

rule2 = {k → √((L - m + 1/2) (L + m + 1/2))}; A1 = ( m - 1/2      k        );
                                                   ( k         -(m + 1/2)  )

eq1 = Eigensystem[A1];

λ1 = eq1[[1, 2]] /. rule1 // Simplify[#, L > 0] &

L

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

-1 - L

f1 = eq1[[2, 2]] /. rule1 // Simplify;
f2 = eq1[[2, 1]] /. rule1 // Simplify;

Normalize[f1] /. rule2 // FullSimplify[#, {L - m + 1/2 > 0, L + m + 1/2 > 0}] &

{√(1/2 + m/(1 + 2 L)), √(1/2 - m/(1 + 2 L))}

Normalize[f2] /. rule2 // FullSimplify[#, {L - m + 1/2 > 0, L + m + 1/2 > 0}] &

{-√(1/2 - m/(1 + 2 L)), √(1/2 + m/(1 + 2 L))}
```

8. Another method (Sakurai)

We start from the assumption that

$$\left| j = l + \frac{1}{2}, m \right\rangle = \alpha\left|\phi_1\right\rangle + \beta\left|\phi_2\right\rangle$$

$$\left| j = l - \frac{1}{2}, m \right\rangle = \gamma\left|\phi_1\right\rangle + \delta\left|\phi_2\right\rangle$$

where we need to determine the values of α, β, γ, and δ. The normalization condition:

$$\alpha^2 + \beta^2 = 1$$

$$\gamma^2 + \delta^2 = 1$$

The condition of the orthogonality:

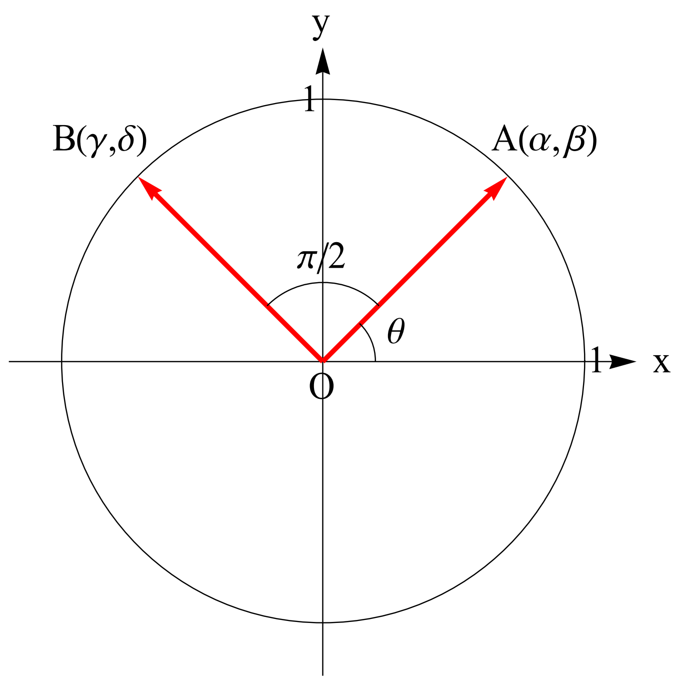
$$\alpha\gamma + \beta\delta = 0$$

There are four unknown parameters and three equations. So we need one more equation. Later, we show that

$$\frac{\alpha}{\beta} = \sqrt{\frac{l+m+\frac{1}{2}}{l-m+\frac{1}{2}}}.$$

We want to determine the values of β, γ, and δ. To this end, we assume that

$$\alpha = \cos\theta,$$
$$\beta = \sin\theta$$
$$\gamma = \cos(\theta + \pi/2) = -\sin\theta, \delta = \sin(\theta + \pi/2) = \cos\theta$$



Since

$$\alpha^2 + \beta^2 = 1,$$

we have

$$\beta = \sqrt{1 - \frac{l+m+\frac{1}{2}}{2l+1}} = \sqrt{\frac{l-m+\frac{1}{2}}{2l+1}} .$$

Then we get

$$\alpha = \delta = \sqrt{\frac{l+m+1/2}{2l+1}} , \qquad \beta = -\gamma = \sqrt{\frac{l-m+1/2}{2l+1}} .$$

where $\alpha > 0$, $\beta > 0$, $\gamma < 0$, and $\delta > 0$ (assumption). The final result is the same as one derived from the Clebsch-Gordan coefficient (addition of angular momentum).

$$\left| j = l+1/2, m \right\rangle = \sqrt{\frac{l+m+1/2}{2l+1}} \left| m_l = m-1/2, m_s = 1/2 \right\rangle + \sqrt{\frac{l-m+1/2}{2l+1}} \left| m_l = m+1/2, m_s = -1/2 \right\rangle$$

$$\left| j = l-1/2, m \right\rangle = -\sqrt{\frac{l-m+1/2}{2l+1}} \left| m_l = m-1/2, m_s = 1/2 \right\rangle + \sqrt{\frac{l+m+1/2}{2l+1}} \left| m_l = m+1/2, m_s = -1/2 \right\rangle$$

or

$$\left| j = l+1/2, m \right\rangle = \begin{pmatrix} \sqrt{\frac{l+m+1/2}{2l+1}} \\ \sqrt{\frac{l-m+1/2}{2l+1}} \end{pmatrix} ,$$

$$\left| j = l-1/2, m \right\rangle == \begin{pmatrix} -\sqrt{\frac{l-m+1/2}{2l+1}} \\ \sqrt{\frac{l+m+1/2}{2l+1}} \end{pmatrix} .$$

((**Note**))

The ratio α/β can be determined as follows. We demand that

$$\hat{\boldsymbol{J}}^2 \left| j = l + \frac{1}{2}, m \right\rangle = \hbar^2 j(j+1) \left| j = l + \frac{1}{2}, m \right\rangle = \hbar^2 (l + \frac{1}{2})(l + \frac{3}{2}) \left| j = l + \frac{1}{2}, m \right\rangle ,$$

where

$$\left| j = l + \frac{1}{2}, m \right\rangle = \alpha \left| m_l = m - \frac{1}{2}, m_s = \frac{1}{2} \right\rangle + \beta \left| m_l = m + \frac{1}{2}, m_s = -\frac{1}{2} \right\rangle .$$

Here we note that

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

Then we get

$$\begin{aligned}\hat{\boldsymbol{J}}^2 \alpha |\phi_1\rangle &= \hbar^2 \alpha [l(l+1) + \frac{3}{4} + (m - \frac{1}{2}) + \hat{L}_+ \hat{S}_-] |\phi_1\rangle \\ &= \hbar^2 \alpha [l(l+1) + \frac{3}{4} + (m - \frac{1}{2}) |\phi_1\rangle + \hbar^2 \alpha \sqrt{(l + m + \frac{1}{2})(l - m + \frac{1}{2})} |\phi_2\rangle\end{aligned}$$

$$\begin{aligned}\hat{\boldsymbol{J}}^2 \beta |\phi_2\rangle &= \hbar^2 \beta [l(l+1) + \frac{3}{4} - (m + \frac{1}{2}) + \hat{L}_- \hat{S}_+] |\phi_2\rangle \\ &= \hbar^2 \beta [l(l+1) + \frac{3}{4} - (m + \frac{1}{2}) |\phi_2\rangle \\ &+ \hbar^2 \beta \sqrt{(l + m + \frac{1}{2})(l - m + \frac{1}{2})} |\phi_1\rangle\end{aligned}$$

Since

$$\hat{\boldsymbol{J}}^2 \left| j = l + \frac{1}{2}, m \right\rangle = \hat{\boldsymbol{J}}^2 (\alpha |\phi_1\rangle + \beta |\phi_2\rangle) = \hbar^2 (l + \frac{3}{2})(l + \frac{1}{2})(\alpha |\phi_1\rangle + \beta |\phi_2\rangle)$$

we have

$$\begin{aligned}&\hbar^2 (l + \frac{1}{2})(l + \frac{3}{2})[\alpha |\phi_1\rangle + \beta |\phi_2\rangle] \\ &= \hbar^2 \alpha [l(l+1) + \frac{3}{4} + (m - \frac{1}{2})] |\phi_1\rangle \\ &+ \hbar^2 \alpha \sqrt{(l + m + \frac{1}{2})(l - m + \frac{1}{2})} |\phi_2\rangle \\ &+ \hbar^2 \beta [l(l+1) + \frac{3}{4} - (m + \frac{1}{2})] |\phi_2\rangle \\ &+ \hbar^2 \beta \sqrt{(l + m + \frac{1}{2})(l - m + \frac{1}{2})} |\phi_1\rangle\end{aligned}$$

or

$$
\begin{aligned}
&[\alpha\sqrt{(l+m+\frac{1}{2})(l-m+\frac{1}{2})}-\beta(l+m+\frac{1}{2})]|\phi_1\rangle \\
&+[\beta\sqrt{(l+m+\frac{1}{2})(l-m+\frac{1}{2})}-\alpha(l-m+\frac{1}{2})]|\phi_2\rangle \\
&=0
\end{aligned}
$$

Then we have

$$\frac{\alpha}{\beta}=\sqrt{\frac{l+m+\frac{1}{2}}{l-m+\frac{1}{2}}}.$$

9. Energy splitting due to the spin-orbit interaction

The eigenket can be described by

$$|\psi\rangle=|j,m;l,s\rangle$$

Note that the expression of the state can be formulated using the Clebsch-Gordan coefficient. When the spin orbit interaction is the perturbation Hamiltonian, we can apply the degenerate theory for the perturbation theory,

$$
\begin{aligned}
\hat{H}_{LS}|\psi\rangle &= \xi\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}|j,m;l,s\rangle \\
&=\xi\frac{1}{2}(\hat{\boldsymbol{J}}^2-\hat{\boldsymbol{L}}^2-\hat{\boldsymbol{S}}^2)|j,m;l,s\rangle \\
&=\frac{\xi\hbar^2}{2}[j(j+1)-l(l+1)-s(s+1)]|j,m;l,s\rangle \\
&=E_{LS}|j,m;l,s\rangle
\end{aligned}
$$

For $j=l+\frac{1}{2}$, $\qquad E_{LS}=E_1=\frac{\xi l\hbar^2}{2}$

For $j=l-\frac{1}{2}$, $\qquad E_{LS}=E_2=-\frac{\xi(l+1)\hbar^2}{2}$

Thus the energy eigenvalue due to the spin-orbit interaction is

$$E_{so} = \frac{\xi\hbar^2}{2}[j(j+1) - l(l+1) - s(s+1)]$$
$$= \frac{e^2\hbar^2}{4m_e^2c^2}\frac{[j(j+1) - l(l+1) - s(s+1)]}{n^3 a_B^3 l(l+1/2)(l+1)}$$
$$= \frac{E_n^2}{m_e c^2}\frac{n[j(j+1) - l(l+1) - s(s+1)]}{l(l+1/2)(l+1)}$$

and the eigenket is $|\psi\rangle = |j,m;l,s\rangle$, where

$$nE_n^2 = \frac{\hbar^2 e^2}{m_e}\frac{1}{4n^3 a_B^3}$$

$$\frac{e^2\hbar^2}{2m_e^2c^2a_B^3} = 7.24524 \text{ x } 10^{-4} \text{ eV}$$

We note that

$$E_{so} = \frac{m_e c^2\alpha^4}{4}\frac{Z^4}{n^3 l(l+\frac{1}{2})(l+1)}\begin{cases} l & j = l+\frac{1}{2} \\ -(l+1) & j = l-\frac{1}{2} \end{cases}$$

with

$$\frac{m_e c^2\alpha^4}{4} = 362.263 \text{ μeV}.$$

We consider the hydrogen atom (1 electron) [spin 1/2, and l] problem with the spin orbit interaction, where $Z = 1$.

The eigenket $|\psi\rangle$ is expressed by $|n,l,s;j,m\rangle$. The angular part of this eigenket is

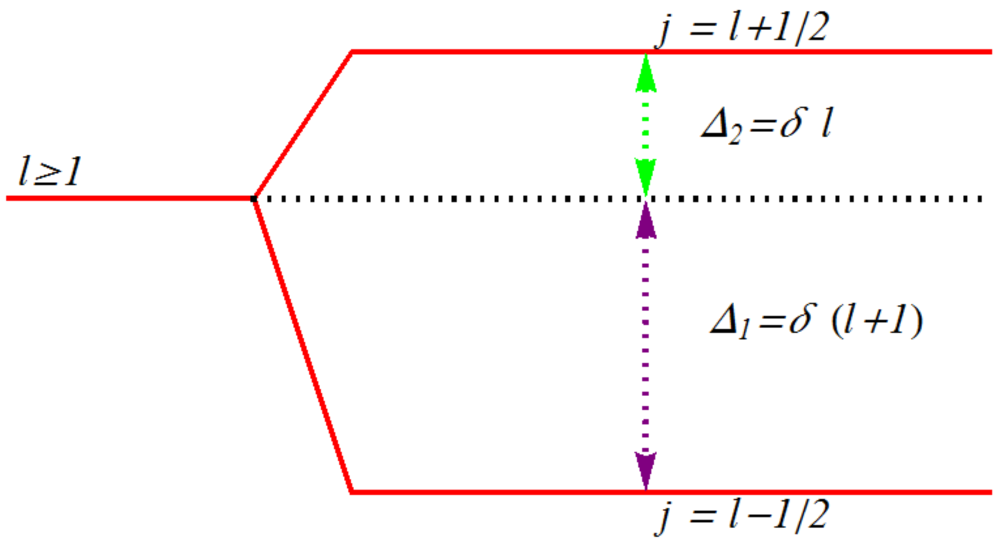
$$|j,m\rangle = |j,m;l,s;\rangle$$

with

$s = 1/2$, $j = l \pm 1/2$

$$\hat{H}_{so} = \xi\hat{L}\cdot\hat{S} = \frac{\xi}{2}(\hat{\boldsymbol{J}}^2 - \hat{\boldsymbol{L}}^2 - \hat{\boldsymbol{S}}^2)$$

$$\hat{H}_{so}|j,m\rangle = \xi\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}|j,m\rangle$$
$$= \frac{\xi}{2}(\hat{\boldsymbol{J}}^2 - \hat{\boldsymbol{L}}^2 - \hat{\boldsymbol{S}}^2)|j,m\rangle$$
$$= \frac{\xi}{2}\hbar^2[j(j+1) - l(l+1) - 3/4]|j,m\rangle$$



((**Note**))
The energy levels with degenerate states are split to the state with $j = l + 1/2$ and the state with $j = l - 1/2$, due to the spin-orbit interaction. However, these states are still degenerate. When the magnetic field is applied to the system, these states are finally separated into the non-degenerate states.

$|j = l + 1/2, m_+\rangle$, where $m_+ = l + 1/2, l - 1/2, \ldots, -(l + 1/2)$

and

$|j = l - 1/2, m_-\rangle$, where $m_- = l - 1/2, l - 3/2, \ldots, -(l - 1/2)$

(a) For $j = l + 1/2$,

$$E_{so} = \frac{\xi}{2}\hbar^2[(l+1/2)(l+3/2) - l(l+1) - 3/4] = \frac{\xi}{2}\hbar^2 l$$

Then we have

$$\left| j = l + 1/2, m \right\rangle = \sqrt{\frac{l + m + 1/2}{2l + 1}} \left| m_l = m - 1/2, m_s = 1/2 \right\rangle + \sqrt{\frac{l - m + 1/2}{2l + 1}} \left| m_l = m + 1/2, m_s = -1/2 \right\rangle$$

In summary, the energy shift due to the spin-orbit interaction is given by

$$E_{so} = \frac{\xi}{2}\hbar^2 l \,, \qquad \text{for } j = l+1/2$$

$$E_{so} = -\frac{\xi}{2}\hbar^2 (l+1) \,, \qquad \text{for } j = l-1/2$$

$$\hat{H}_{so} = \begin{pmatrix} \frac{\xi}{2}\hbar^2 l & 0 \\ 0 & -\frac{\xi}{2}\hbar^2 (l+1) \end{pmatrix}$$

under the basis of $\left| j = l + 1/2, m \right\rangle$ and $\left| j = l - 1/2, m \right\rangle$, where

$$\frac{\hbar^2 \xi}{\left| E_n \right|} = \frac{e^4}{c^2 n^2 \hbar^2 l(l+1/2)(l+1)} = \frac{\alpha^2}{n^2} \frac{1}{l(l+1/2)(l+1)}$$

or

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

10. The Zeeman splitting

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

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

We now consider the influence of the magnetic field on the eigenstates $\left| j = l + 1/2, m \right\rangle$ and $\left| j = l - 1/2, m \right\rangle$

(a) $\left| j = l + 1/2, m \right\rangle$

$$\hat{H}_{so}\left| j = l + 1/2, m \right\rangle = \frac{\xi}{2}\hbar^2 l \left| j = l + 1/2, m \right\rangle$$

The expectation value of $\hat{L}_z$ and $\hat{S}_z$

$$\hat{L}_z \left| j = l + 1/2, m \right\rangle = \hbar\sqrt{\frac{l + m + 1/2}{2l + 1}}(m - 1/2)\left| m_l = m - 1/2, m_s = 1/2 \right\rangle + \hbar\sqrt{\frac{l - m + 1/2}{2l + 1}}(m + 1/2)\left| m_l = m + 1/2, m_s = -1/2 \right\rangle$$

$$\begin{aligned}\left\langle j = l + 1/2, m \right| \hat{L}_z \left| j = l + 1/2, m \right\rangle &= \hbar \begin{pmatrix} \sqrt{\frac{l + m + 1/2}{2l + 1}} & \sqrt{\frac{l - m + 1/2}{2l + 1}} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{l + m + 1/2}{2l + 1}}(m - 1/2) \\ \sqrt{\frac{l - m + 1/2}{2l + 1}}(m + 1/2) \end{pmatrix} \\ &= \hbar\left[\frac{l + m + 1/2}{2l + 1}(m - 1/2) + \frac{l - m + 1/2}{2l + 1}(m + 1/2)\right] \\ &= \frac{\hbar 2lm}{2l + 1}\end{aligned}$$

Similarly,

$$\hat{S}_z \left| j = l + 1/2, m \right\rangle = \hbar\sqrt{\frac{l + m + 1/2}{2l + 1}}(1/2)\left| m_l = m - 1/2, m_s = 1/2 \right\rangle + \hbar\sqrt{\frac{l - m + 1/2}{2l + 1}}(-1/2)\left| m_l = m + 1/2, m_s = -1/2 \right\rangle$$

$$\begin{aligned}\left\langle j = l + 1/2, m \right| \hat{S}_z \left| j = l + 1/2, m \right\rangle &= \hbar\left[\frac{l + m + 1/2}{2l + 1}(1/2) - \frac{l - m + 1/2}{2l + 1}(1/2)\right] \\ &= \frac{\hbar m}{2l + 1}\end{aligned}$$

Then we have the expectation value of $\hat{H}_B$ as

$$
\begin{aligned}
E_{B1} &= \langle j=l+1/2,m|\hat{H}_B|j=l+1/2,m\rangle \\
&= \langle j=l+1/2,m|\hat{L}_z+2\hat{S}_z|j=l+1/2,m\rangle \\
&= \frac{\mu_B B}{\hbar}\hbar m(1+\frac{1}{2l+1}) \\
&= m\mu_B B(1+\frac{1}{2l+1}) \\
&= 2m\mu_B B\left(\frac{l+1}{2l+1}\right)
\end{aligned}
$$

(b) For $j = l$ -1/2,

$$E_{LS} = \frac{\xi}{2}\hbar^2[(l-\frac{1}{2})(l+\frac{1}{2})-l(l+1)-\frac{3}{4}] = -\frac{\xi}{2}\hbar^2(l+1)$$

$$
\begin{aligned}
|j=l-1/2,m\rangle = &-\sqrt{\frac{l-m+1/2}{2l+1}}|m_l=m-1/2,m_s=1/2\rangle \\
&+\sqrt{\frac{l+m+1/2}{2l+1}}|m_l=m+1/2,m_s=-1/2\rangle
\end{aligned}
$$

or

$$\hat{H}_{so}|j=l-1/2,m\rangle = -\frac{\xi}{2}\hbar^2(l+1)|j=l-1/2,m\rangle$$

The expectation value of $\hat{L}_z$ and $\hat{S}_z$

$$
\begin{aligned}
\langle j=l-1/2,m|\hat{L}_z|j=l-1/2,m\rangle &= \hbar\left[\frac{l-m+1/2}{2l+1}(m-1/2)+\frac{l+m+1/2}{2l+1}(m+1/2)\right] \\
&= \frac{2\hbar m(l+1)}{2l+1}
\end{aligned}
$$

$$
\begin{aligned}
\langle j=l-1/2,m|\hat{S}_z|j=l-1/2,m\rangle &= \hbar\left[\frac{l-m+1/2}{2l+1}(1/2)-\frac{l+m+1/2}{2l+1}(1/2)\right] \\
&= -\frac{\hbar m}{2l+1}
\end{aligned}
$$

$$\langle j=l-1/2,m|\hat{L}_z+2\hat{S}_z|j=l-1/2,m\rangle = \hbar m(1-\frac{1}{2l+1})$$

Then we have the expectation value of $\hat{H}_B$ as

$$
\begin{aligned}
E_{B2} &= \langle j=l-1/2, m|\hat{H}_B|j=l-1/2, m\rangle \\
&= \langle j=l-1/2, m|\hat{L}_z + 2\hat{S}_z|j=l-1/2, m\rangle \\
&= \frac{\mu_B B}{\hbar}\hbar m(1-\frac{1}{2l+1}) \\
&= 2m\mu_B B(\frac{1}{2l+1})
\end{aligned}
$$

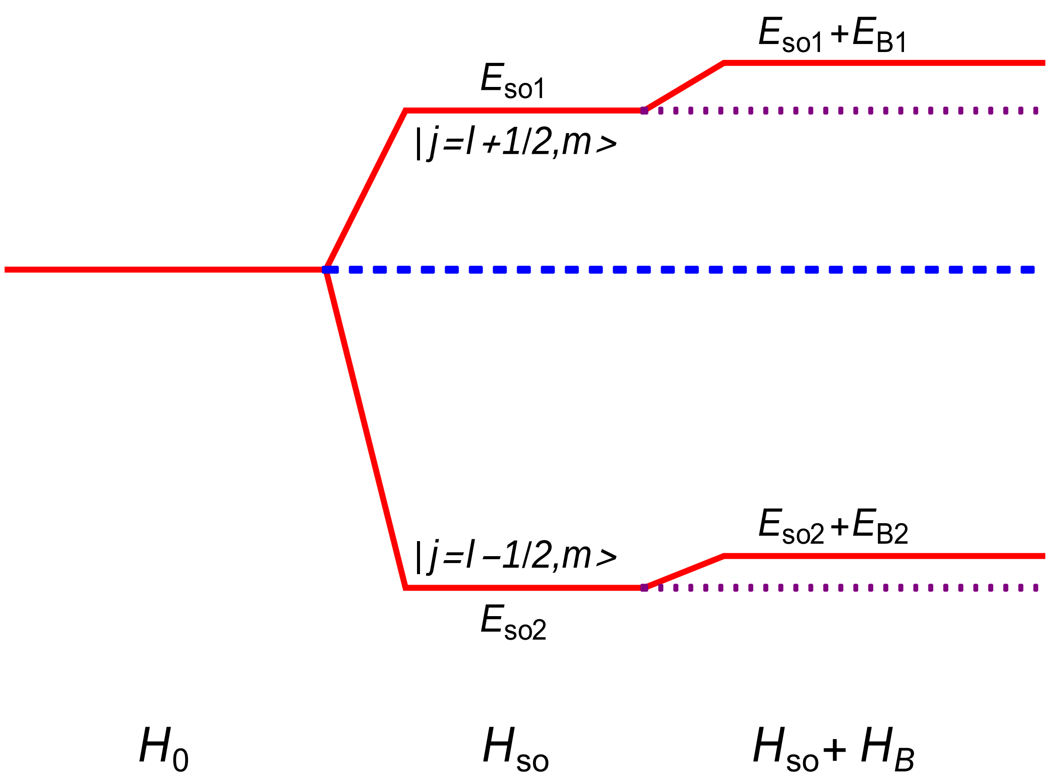


Fig. Energy level splitting due to the spin orbit interaction and the Zeeman effect

$E_{so1} = \frac{\xi}{2}\hbar^2 l$, $E_{so2} = -\frac{\xi}{2}\hbar^2(l+1)$, $E_{B1} = 2m\mu_B B\left(\frac{l+1}{2l+1}\right)$, and

$E_{B2} = 2m\mu_B B(\frac{1}{2l+1})$

11. Effect of the spin-orbit interaction on the spectrum in hydrogen atom

For hydrogen, Z = 1.

$$E_{SO} = \frac{\xi}{2}(\boldsymbol{J}^2 - \boldsymbol{L}^2 - \boldsymbol{S}^2) = \frac{\xi\hbar^2}{2}[j(j+1) - l(l+1) - s(s+1)]$$
$$= \frac{m_e c^2}{2}\frac{\alpha^4}{n^3}\frac{[j(j+1) - l(l+1) - s(s+1)]}{l(l+1)(2l+1)}$$

where α is the fine structure

$$\alpha = \frac{e^2}{\hbar c} = \frac{1}{137.036} = 7.2973525698 \text{ x } 10^{-3}$$

(a) The energy level of the 2S state does not change since $L = 0$.
(b) The 2P state is split into two states due to the spin-orbit coupling.

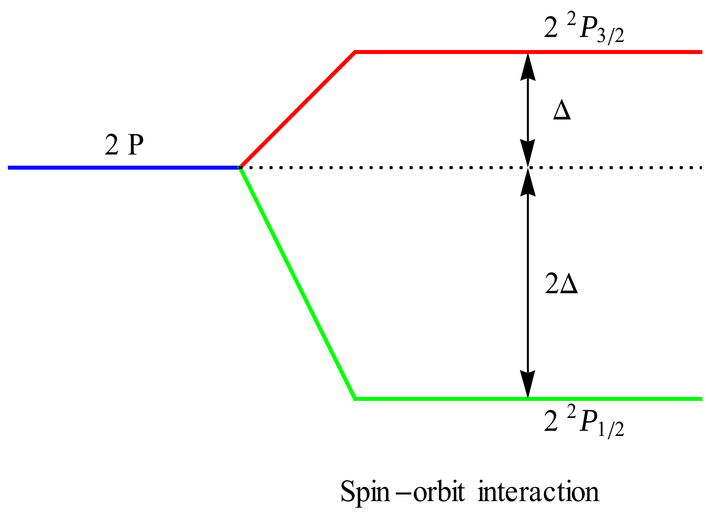


Fig. Splitting of 2 P level into two states (2 $^2P_{3/2}$ and 2 $^2P_{1/2}$).

$l = 1$ (2p) and spin s = 1/2 $\rightarrow j = 3/2$ and $j = 1/2$

($D_1 \times D_{1/2} = D_{3/2} + D_{1/2}$).

2 $^2P_{3/2}$ ($j = 3/2$, $l = 1$, $s = 1/2$)

2 $^2P_{1/2}$ ($j = 1/2$, $l = 1$, $s = 1/2$)

When s = 1/2,

$E_{SO} = \Delta = 15.0943\ \mu$eV for the 2 $^2P_{3/2}$ state

$E_{SO} = -2\Delta = -30.1886\ \mu$eV for the 2 $^2P_{1/2}$ state

$$3\Delta = 45.2829 \ \mu\text{eV}.$$

The energy difference is $3\Delta = 45.2829$ μeV.

Note that the Landè g-factor is defined by.

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

For $^2P_{3/2}$ ($j = 3/2$, $l = 1$, $s = 1/2$)

$$g_1 = \frac{3}{2} + \frac{\frac{3}{4} - 1(1+1)}{2\frac{3}{2}\frac{5}{2}} = \frac{4}{3}.$$

For $^2P_{1/2}$ ($j = 1/2$, $l = 1$, $s = 1/2$)

$$g_2 = \frac{3}{2} + \frac{\frac{3}{4} - 1(1+1)}{2\frac{1}{2}\frac{3}{2}} = \frac{2}{3}.$$

(c) The 3p state is split into two states due to the spin-orbit coupling.

$l = 1$ (3p) and spin $s = 1/2 \rightarrow j = 3/2$ and $j = 1/2$

($D_1 \text{ x } D_{1/2} = D_{3/2} + D_{1/2}$).

$3\ ^2P_{3/2}$ ($j = 3/2$, $l = 1$, $s = 1/2$)

$3\ ^2P_{1/2}$ ($j = 1/2$, $l = 1$, $s = 1/2$)

Then we have

$E_{SO} = \Delta = 4.47239$ μeV for the $3\ ^2P_{3/2}$ state

$E_{SO} = -2\Delta = -8{,}94478$ μeV for the $3\ ^2P_{1/2}$ state

$$3\Delta = 13.4172 \ \mu\text{eV}.$$

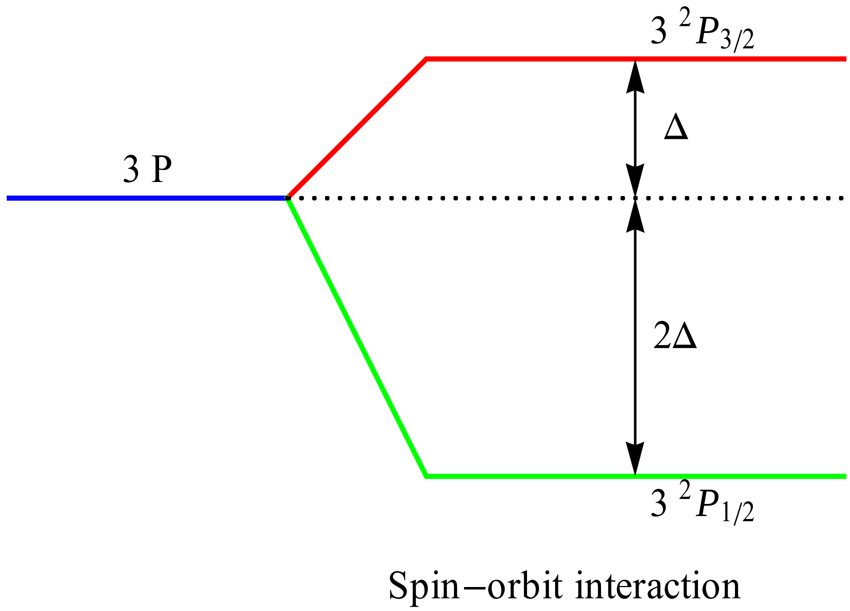


Fig. Splitting of 3 P level into two states ($3\ ^2P_{3/2}$ and $3\ ^2P_{1/2}$)

$E_{SO} = \Delta = 4.47239$ μeV for the $3\ ^2P_{3/2}$ state

$E_{SO} = -2\Delta = -8.94478$ μeV for the $3\ ^2P_{1/2}$ state

$3\Delta = 13.4172\ \mu$eV.

(d) We note that the energy level of the 3S state does not change since $L = 0$.

---

12. Sodium D lines

The electron configuration of Na is $(1s)^2(2s)^2(2p)^6(3s)^1$. The atomic number is Z = 11. The famous Na doublet arises from the spin-orbit splitting of Na 3p level, and consists of the closely spaced pair of spectral lines at wavelength of D_1 line (589.592 nm) for the transition $3\ ^2P_{1/2} \rightarrow 3\ ^2S_{1/2}$, and D_2 line (588.995 nm) $^2P_{3/2} \rightarrow {}^2S_{1/2}$. (Serway).

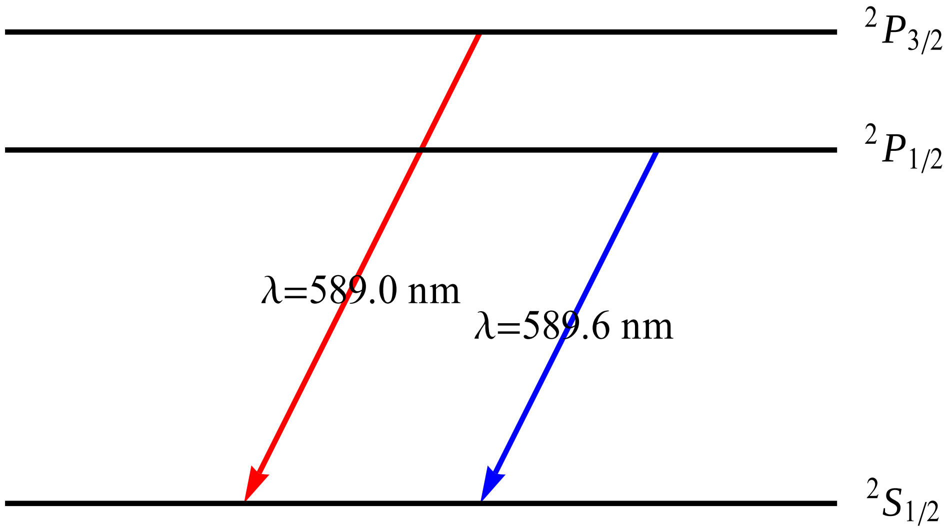


Fig. 3 $^2P_{3/2}$ (j = 3/2, l = 1, s = 1/2). 3 $^2P_{1/2}$ (j = 1/2, l = 1, s = 1/2). 3 $^2S_{1/2}$ (j = 1/2, l = 0, s = 1/2). The splitting of the energy levels (3 $^2P_{3/2}$ and the 3 $^2P_{1/2}$) is due to the spin-orbit interaction. The D_1 line (denoted by blue line). The D_2 line (denoted by red line).

The sodium D lines correspond to the 3p → 3s transition. In the absence of a magnetic field B, the spin orbit interaction splits the upper 3p state into 3 $^2P_{3/2}$ and 3 $^2P_{1/2}$ terms separated by 17 cm^{-1}. The lower 3 $^2S_{1/2}$ has no spin-orbit interaction.
For l = 1, the energy shift due to the spin-orbit interaction is given by

$$E_{s0} = \Delta, \qquad \text{for } j = 3/2 \qquad (3\ ^2P_{3/2})$$

$$E_{so} = -2\Delta, \qquad \text{for } j = 1/2 \qquad (3\ ^2P_{1/2})$$

For the Na doublet, the observed wavelength difference is

$$\Delta\lambda = \lambda_2 - \lambda_1 = 0.597\ \text{nm},$$

since

$$\lambda_2 = 589.592\ \text{nm}, \qquad \lambda_1 = 588.995\ \text{nm}.$$

Then the energy difference between the 3 $^2P_{3/2}$ state and 3 $^2P_{1/2}$ state is derived as follows.

$$\Delta E = 3\Delta = \frac{hc}{\lambda_1\lambda_2}\Delta\lambda = 2.1314 \times 10^{-3}\ \text{eV}$$

13. Clebsch-Gordan co-efficient in Na

(a) For the electron with 3s state ($l = 0$, $s = 1/2$)

$D_0 \times D_{1/2} = D_{1/2}$

Thus we have $j = 1/2$. The state is described by $^2S_{1/2}$.

$$\left| j = 1/2, m = 1/2 \right\rangle = \left| m_l = 0, m_s = 1/2 \right\rangle$$

$$\left| j = 1/2, m = -1/2 \right\rangle = \left| m_l = 0, m_s = -1/2 \right\rangle$$

(b) For the electron with 3p state ($l = 1$, $s = 1/2$)

$D_1 \times D_{1/2} = D_{3/2} + D_{1/2}$

Thus we have $j = 3/2$ and $j = 1/2$. The state is described by $^2P_{3/2}$ and $^2P_{1/2}$

(i) $j = 3/2$

$$\left| j = 3/2, m = -3/2 \right\rangle = \left| m_l = -1, m_s = -1/2 \right\rangle$$

$$\left| j = 3/2, m = -1/2 \right\rangle = \sqrt{\frac{2}{3}} \left| m_l = 0, m_s = -1/2 \right\rangle + \frac{1}{\sqrt{3}} \left| m_l = -1, m_s = 1/2 \right\rangle$$

$$\left| j = 3/2, m = 1/2 \right\rangle = \frac{1}{\sqrt{3}} \left| m_l = 1, m_s = -1/2 \right\rangle + \sqrt{\frac{2}{3}} \left| m_l = 0, m_s = 1/2 \right\rangle$$

$$\left| j = 3/2, m = 3/2 \right\rangle = \left| m_l = 1, m_s = 1/2 \right\rangle$$

(ii) $j = 1/2$

$$\left| j = 1/2, m = -1/2 \right\rangle = \frac{1}{\sqrt{3}} \left| m_l = 0, m_s = -1/2 \right\rangle - \sqrt{\frac{2}{3}} \left| m_l = -1, m_s = 1/2 \right\rangle$$

$$\left| j = 1/2, m = 1/2 \right\rangle = \sqrt{\frac{2}{3}} \left| m_l = 1, m_s = -1/2 \right\rangle - \frac{1}{\sqrt{3}} \left| m_l = 0, m_s = 1/2 \right\rangle$$

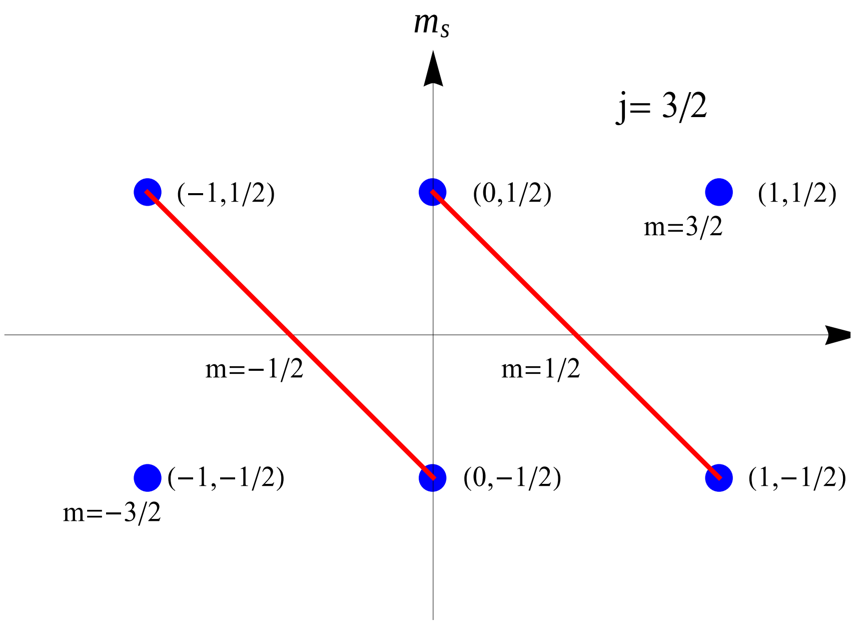


Fig. Clebsh-Gordan diagram for $|j,m\rangle$ with j = 3/2. m = 3/2, 1/2, -1/2, and -3/2.

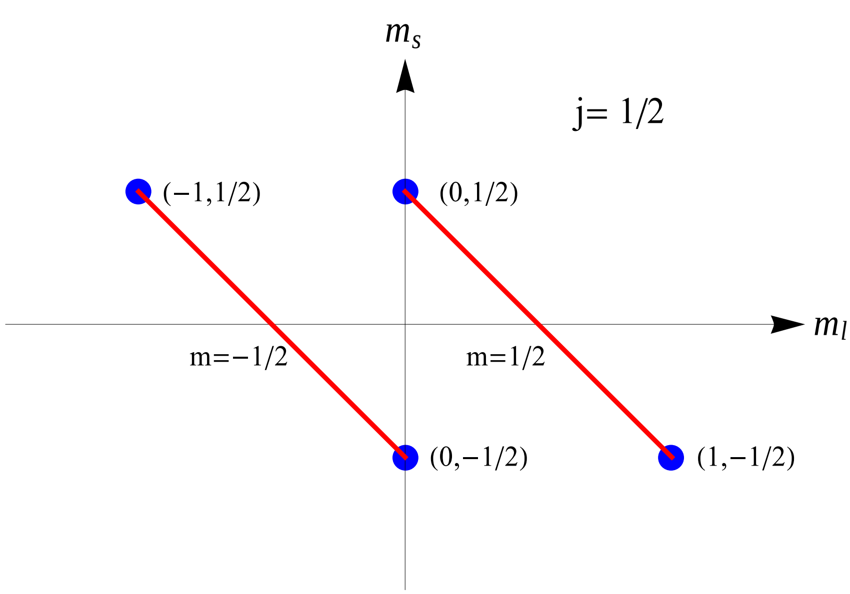


Fig. Clebsh-Gordan diagram for $|j,m\rangle$ with j = 1/2. m = 1/2 and -1/2.

14. Total angular momentum and the total 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 Landé g-factor is defined by

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

where

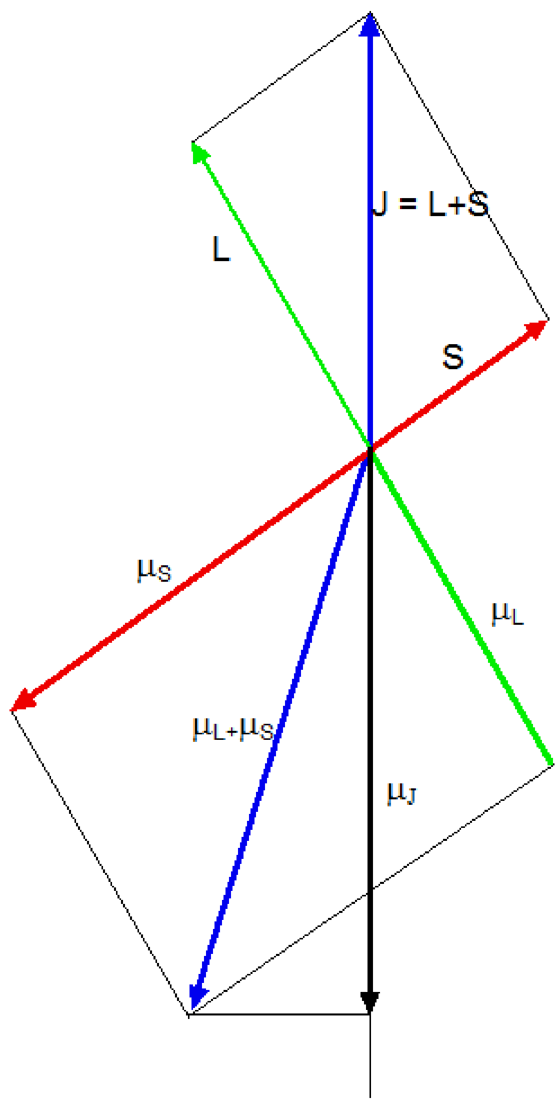


Fig. Basic classical vector model of orbital angular momentum (***L***), spin angular momentum (***S***), orbital magnetic moment ($\boldsymbol{\mu}_L$), and spin magnetic moment ($\boldsymbol{\mu}_S$). ***J*** (= ***L*** + ***S***) is the total angular momentum. $\boldsymbol{\mu}_J$ is the component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

Suppose that

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

where a and b are constants, and the vectors $\boldsymbol{S}_\perp$ and $\boldsymbol{L}_\perp$ are perpendicular to $\boldsymbol{J}$.
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 the Landé g-factor

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

15. Landé *g*-factor in Na

The Landé *g*-factor is given by

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

Table

Term	j	l	S	g
$2\ ^2P_{3/2}$	3/2	1	1/2	4/3
$2\ ^2P_{1/2}$	1/2	1	1/2	2/3

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APPENDIX-I Clebsch-Gordan co-efficient

Mathematica program for the Clebsch-Gordan coefficients

```
Clear["Global`*"];

CCGG[{j1_, m1_}, {j2_, m2_}, {j_, m_}] :=
 Module[{s1},
  s1 = If[Abs[m1] ⩽ j1 && Abs[m2] ⩽ j2 && Abs[m] ⩽ j,
    ClebschGordan[{j1, m1}, {j2, m2}, {j, m}], 0]]

CG[{j_, m_}, j1_, j2_] :=
 Sum[CCGG[{j1, m1}, {j2, m - m1}, {j, m}] a[j1 , m1]
   b[j2,  m - m1], {m1, -j1, j1}]
```

j1 = 1 and j2 = 1/2;

```
j1 = 1; j2 = 1 / 2;

CG[{3 / 2, 3 / 2}, j1, j2]
```

$a[1,1]\, b\left[\frac{1}{2}, \frac{1}{2}\right]$

```
CG[{3 / 2, 1 / 2}, j1, j2]
```

$\frac{a[1,1]\, b\left[\frac{1}{2}, -\frac{1}{2}\right]}{\sqrt{3}} + \sqrt{\frac{2}{3}}\, a[1,0]\, b\left[\frac{1}{2}, \frac{1}{2}\right]$

```
CG[{3/2, -1/2}, j1, j2]
```

$$\sqrt{\frac{2}{3}}\, a[1,0]\, b\left[\frac{1}{2}, -\frac{1}{2}\right] + \frac{a[1,-1]\, b\left[\frac{1}{2}, \frac{1}{2}\right]}{\sqrt{3}}$$

```
CG[{3/2, -3/2}, j1, j2]
```

$$a[1,-1]\, b\left[\frac{1}{2}, -\frac{1}{2}\right]$$

```
CG[{1/2, 1/2}, j1, j2]
```

$$\sqrt{\frac{2}{3}}\, a[1,1]\, b\left[\frac{1}{2}, -\frac{1}{2}\right] - \frac{a[1,0]\, b\left[\frac{1}{2}, \frac{1}{2}\right]}{\sqrt{3}}$$

```
CG[{1/2, -1/2}, j1, j2]
```

$$\frac{a[1,0]\, b\left[\frac{1}{2}, -\frac{1}{2}\right]}{\sqrt{3}} - \sqrt{\frac{2}{3}}\, a[1,-1]\, b\left[\frac{1}{2}, \frac{1}{2}\right]$$

j1 = 0 and j2 = 1/2

```
j1 = 0; j2 = 1/2;
```

```
CG[{1/2, 1/2}, j1, j2]
```

$$a[0,0]\, b\left[\frac{1}{2}, \frac{1}{2}\right]$$

```
CG[{1/2, -1/2}, j1, j2]
```

$$a[0,0]\, b\left[\frac{1}{2}, -\frac{1}{2}\right]$$

APPENDIX-II Effect of spin orbit interaction of 2p electron

Application of the perturbation theory (degenerate case)

We consider the state of 2p electron. Suppose that there is one electron with spin 1/2. There are 6 states, taking into account of spin 1/2. These are degenerate states

The orbital angular momentum:

$l = 1$ (p state) $\qquad$ (m_l = 1, 0, -1)

The spin angular momentum: $s = \dfrac{1}{2}$ $\qquad$ (m_s = 0)

The total angular momentum:

$$D_1 \times D_{1/2} = D_{3/2} + D_{1/2}$$

leading to

$$j = \frac{3}{2} \qquad (m = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2})$$

$$j = \frac{1}{2} \qquad (m = \frac{1}{2}, -\frac{1}{2})$$

The degenerate state for 2p statefor the unperturbed Hamiltonian

(a) The unperturbed state:

There are 6 states: 3 x 2 = 6:

(i) $j = \frac{3}{2}$ ($2\,^2P_{3/2}$ state)

$$\left| j = \frac{3}{2}, m = \frac{3}{2}, l = 1, s = \frac{1}{2} \right\rangle$$

$$\left| j = \frac{3}{2}, m = \frac{1}{2}, l = 1, s = \frac{1}{2} \right\rangle$$

$$\left| j = \frac{3}{2}, m = -\frac{1}{2}, l = 1, s = \frac{1}{2} \right\rangle$$

$$\left| j = \frac{3}{2}, m = -\frac{3}{2}, l = 1, s = \frac{1}{2} \right\rangle$$

(ii) $j = \frac{1}{2}$ ($2\,^2P_{1/2}$ state)

$$\left| j = \frac{1}{2}, m = \frac{1}{2}, l = 1, s = \frac{1}{2} \right\rangle$$

$$\left| j = \frac{1}{2}, m = -\frac{1}{2}, l = 1, s = \frac{1}{2} \right\rangle$$

(b) Perturbed states

According to the perturbation theory, we have

$$\begin{aligned}\hat{H}_{LS}|j,m;l,s\rangle &= \xi\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}|j,m;l,s\rangle \\ &= \xi\frac{1}{2}(\hat{\boldsymbol{J}}^2-\hat{\boldsymbol{L}}^2-\hat{\boldsymbol{S}}^2)|j,m;l,s\rangle \\ &= \frac{\xi\hbar^2}{2}[j(j+1)-l(l+1)-s(s+1)]|j,m;l,s\rangle \\ &= E_{LS}|j,m;l,s\rangle\end{aligned}$$

where

$$E_{LS}=\frac{\xi\hbar^2}{2}[j(j+1)-l(l+1)-s(s+1)]$$

So the state $|j,m;l,s\rangle$ is the eigenstate of $\hat{H}_{LS}$. We note that $|j,m;l,s\rangle$ is expressed as

$$|j,m;l,s\rangle=\alpha\left|m_l=m-\frac{1}{2},m_s=\frac{1}{2}\right\rangle+\beta\left|m_l=m+\frac{1}{2},m_s=-\frac{1}{2}\right\rangle$$

where α and β are the Clebsch-Gordan coefficient

For $j=\frac{3}{2}$ $(2\,^2P_{3/2})$ $\quad E_{LS}=\frac{\xi\hbar^2}{2}$. For $j=\frac{1}{2}$ $(2\,^2P_{1/2})$ $\quad E_{LS}=-\xi\hbar^2$