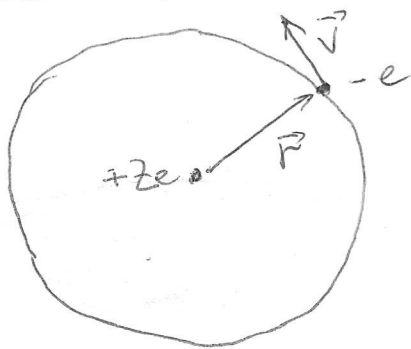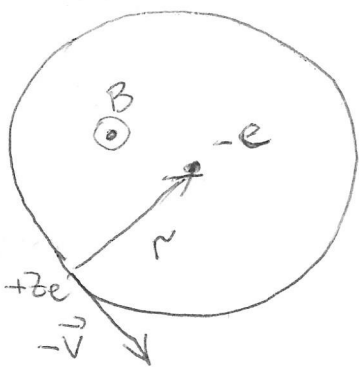# Spin-orbit interaction

We want to consider the interaction between an electron's spin (and magnetic moment associated with it) and the internal magnetic field of a one-electron atom. This internal magnetic field is related to the orbital motion of the electron. This interaction is called the spin-orbit interaction. As we will see, it is a subtle effect in small atoms ($Z \sim 1$). By using the perturbation theory we aim to investigate how this interaction affects the energy levels.

Let us consider the motion of of the nucleus in the reference frame where the electron is at rest.

In this case the electron is located inside a current loop created by the motion of a charged nucleus.

According to the Biot-Savart law

$$\vec{B}(\vec{r}) = \frac{\mu_0}{4\pi} \int_C \frac{I \, d\vec{\ell} \times \vec{r}}{|\vec{r}|^3}$$

In the case of a circular orbit we can easily determine that

$$B = \frac{\mu_0}{4\pi} \cdot \frac{I \cdot 2\pi r \cdot r}{r^3} = \frac{\mu_0 I}{2r}$$

The effective current is given by $I = \frac{Ze}{T}$ where T is the period of the orbit.

At the same time the orbital angular momentum of the electron (in the reference frame where the nucleus is

at rest) is :

$$L = rmv = rm\frac{2\pi r}{T} = \frac{2\pi m r^2}{T}$$

As both $\vec{B}$ and $\vec{L}$ have the same direction we can write that

$$B = \frac{\mu_0 Ze}{2rT} \quad \text{or} \quad \vec{B} = \frac{\mu_0 Ze}{2r}\frac{\vec{L}}{2\pi m r^2} = \frac{\mu_0 Ze}{4\pi m r^3}\vec{L},$$

or, since $\mu_0 \varepsilon_0 = \frac{1}{c^2}$, $\quad \vec{B} = \frac{Ze}{4\pi\varepsilon_0 r^3}\frac{1}{mc^2}\vec{L}$

In a more general case, when, instead of a pure Coulomb attraction between an electron and proton we have some screened potential $V(r)$ the latter expression would become (assuming $V(r)$ to be spher. symmetric)

$$\vec{B} = \frac{1}{emc^2}\frac{1}{r}\frac{dV}{dr}\vec{L}$$

Further, as we know, the interaction of a magnetic moment with field $\vec{B}$ is given by

$$-\vec{\mu}\cdot\vec{B}$$

We also know from the previous semester that the relation between the electron's magnetic moment and spin is

$$\vec{\mu} = -\frac{e}{m}\vec{S}$$

With that the the formula for the interaction energy becomes

$$\frac{e}{m}\vec{B}\cdot\vec{S} = \frac{Ze^2}{4\pi\varepsilon_0 r^3}\frac{1}{m^2c^2}\vec{L}\cdot\vec{S}$$

This energy has been evaluated in the reference frame where the electron is at rest. Because of an effect of the relativistic transformation of the velocities,

called Thomas precession the transformation back to the nuclear rest frame results in an additional factor of $\frac{1}{2}$. Therefore, the Hamiltonian that describes the spin-orbit interaction looks as follows:

$$H'_{so} = \frac{Ze^2}{8\pi\varepsilon_0 m^2 c^2} \frac{1}{r^3} \vec{L}\cdot\vec{S}$$

If we add H'_{so} to the unperturbed Hamiltonian H^0 then the total Hamiltonian will no longer commutes with $\vec{L}$ or $\vec{S}$:

$$[\vec{L}\cdot\vec{S}, L_x] = [L_xS_x + L_yS_y + L_zS_z, L_x] = S_x\underbrace{[L_x,L_x]}_{0} + S_y[L_y,L_x] +$$

$$+ S_z[L_z,L_x] = S_y(-i\hbar L_z) + S_z(i\hbar L_y) = i\hbar(L_yS_z - L_zS_y) = i\hbar(\vec{L}\times\vec{S})_x$$

$$[\vec{L}\cdot\vec{S}, S_x] \overset{L\rightleftarrows S}{=\!=\!=} i\hbar(\vec{S}\times\vec{L})_x$$

However $[\vec{L}\cdot\vec{S}, L_x + S_x] = 0$

So H will commute with $\vec{J} = \vec{L} + \vec{S}$

Since L^2 commutes with all components of $\vec{L}$ and $\vec{S}$ $[H, L^2] = 0$. Likewise $[H, S^2] = 0$

What this means is that neither $\vec{L}$ nor $\vec{S}$ are conserved quantities. (although L^2 and S^2 are). Instead we have a new integral of motion — $\vec{J}$ — the total angular momentum.

What follows from the above fact is that the perturbation matrix is not diagonal in the eigenstates of H^0, L^2, S^2, L_z, S_z. In order to use the simple first order perturbation theory expressions ($E_n^{(1)} = \langle H'\rangle_n$) we need to find the proper basis. Such a basis is

formed by the simultaneous eigenfunctions of

$$H^0, L^2, S^2, J^2, \text{ and } J_z$$

Given simultaneous eigenfunctions of L^2, S^2, L_z, S_z we can construct eigenfunctions of L^2, S^2, J^2, J_z using the coefficients of vector addition (i.e. Clebsch-Gordan coefficients):

$$|\phi\rangle \equiv |n\ell\rangle |jm; \ell s\rangle = |n\ell\rangle \sum_{\substack{m_\ell, m_s \\ m_\ell + m_s = m_j}} C_{m_\ell m_s} |\ell m_\ell\rangle |s m_s\rangle$$

where $|n\ell\rangle$ is the radial component of the hydrogen wave functions, i.e. $H^0 |n\ell\rangle |\ell m\rangle = E_n^{(0)} |n\ell\rangle |\ell m\rangle$

Computing the expectation values of the $\vec{L}\cdot\vec{S}$ operator with the above eigenfunctions of L^2, S^2, J^2, J_z is actually very easy if we recall that

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

which gives

$$\vec{L}\cdot\vec{S} = \tfrac{1}{2}(J^2 - L^2 - S^2)$$

When operator $\vec{L}\cdot\vec{S}$ acts on eigenfunctions of L^2, S^2, J^2, J_z it gives

$$\vec{L}\cdot\vec{S}|\phi\rangle = \hbar^2 \tfrac{1}{2}\left[j(j+1) - \ell(\ell+1) - s(s+1)\right]|\phi\rangle$$

All that remains to be done is to evaluate

$$\langle\phi|\tfrac{1}{r^3}|\phi\rangle = \langle n\ell|\tfrac{1}{r^3}|n\ell\rangle$$

The matrix elements of $\frac{1}{r^3}$ are readily available in many textbooks and internet sources:

$$\left\langle\tfrac{1}{r^3}\right\rangle_{n\ell} = \frac{1}{\ell(\ell+\tfrac{1}{2})(\ell+1)n^3 a^3}$$

(a is the Bohr radius)

With that we can write $E_{so}^{(1)}$:

$$E_{so}^{(1)} = \langle H_{so}' \rangle = \frac{Ze^2}{8\pi\varepsilon_0} \frac{1}{m^2c^2} \frac{\frac{\hbar^2}{2}\left[j(j+1) - \ell(\ell+1) - s(s+1)\right]}{\ell(\ell+\frac{1}{2})(\ell+1) \, n^3 a^3}$$

Since $s = \frac{1}{2}$ for possible values of j we have $j = \ell \pm \frac{1}{2}$

The last formula can be rewritten as

$$E_{so}^{(1)} = \frac{(E_n^{(0)})^2}{mc^2}\left[n \frac{j(j+1) - \ell(\ell+1) - s(s+1)}{\ell(\ell+\frac{1}{2})(\ell+1)} \right]$$

If we combine this result with the one we obtained previously for the relativistic correction we will get a complete correction for the fine structure of hydrogen:

$$E_{fs}^{(1)} = \frac{(E_n^{(0)})^2}{2mc^2}\left(3 - \frac{4n}{j+\frac{1}{2}} \right)$$

and the total energy of the hydrogen then becomes

$$E_{nj} = E_n^{(0)}\left[1 + \frac{\alpha^2}{n^2}\left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4} \right) \right]$$

α is the fine structure constant

i.e. the energy levels depend not only on n but on n and j quantum numbers — the degeneracy is partially lifted.