

Spin orbital coupling in Hydrogen-like atom

So far we ignored the spin of electron and magnetic dipole moment ($\vec{\mu}$) associated with it.

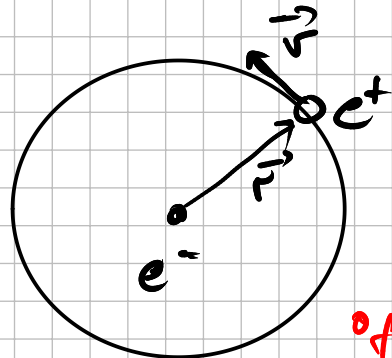
If we have surrounding magnetic field \vec{B} we would have energy term of such interaction

$$H = -\vec{\mu} \cdot \vec{B} \quad \text{simple classical physics.}$$

↑ do not confuse with reduced mass (μ)

If \vec{B} external, we have Zeeman effect (we will cover it soon)

But there is also internal \vec{B} field generated by apparent motion of proton in the electron rest frame.



Biot-Savart law (Phys 102)

$$|\vec{B}| = \frac{\mu_0 I}{2r} = \frac{\mu_0 q v}{2r} = \frac{\mu_0 e Z v}{2r} \cdot \frac{r}{r} \cdot \frac{m_e}{m_e}$$

permeability of free space (yet another μ :))

$$B = \frac{\mu_0 Z e}{4\pi r^3 m_e} \underbrace{m_e r v}_{\substack{= L \text{ - angular momentum} \\ \vec{L} = m_e \vec{r} \times \vec{v}}}$$

$$\Rightarrow \vec{B} = \frac{\mu_0 Z e}{4\pi m_e} \frac{1}{r^3} \vec{L}$$

recall that $\sqrt{\epsilon_0 \mu_0} = 1/c$

$$\vec{B} = \frac{1}{4\pi \epsilon_0} \frac{Z e}{m_e c^2} \frac{1}{r^3} \vec{L} \Rightarrow \boxed{\vec{B} = \frac{1}{4\pi \epsilon_0} \frac{Z e}{m_e c^2} \frac{1}{r^3} \vec{L}}$$

What about magnetic dipole momentum of electron?

$$\vec{M} = \underbrace{A}_{\text{area}} \cdot \underbrace{I}_{\text{radius of electron!}} \sim \underbrace{\pi r^2}_{\text{area of electron is tricky}} \cdot \left(-\frac{e}{t}\right) \sim \pi r^2 \cdot (-e) \cdot \underbrace{\frac{v}{2\pi r} \cdot \frac{m_e}{m_e} \cdot \frac{r}{r}}_{\sim S}$$

actually $\mu = g \cdot \frac{e}{2m_e} \vec{S}$
where $g = 2.002 \dots$

classical estimate $\vec{M} \sim \frac{-e}{2m} \vec{S}$ \Rightarrow the real value

$$\boxed{\vec{M} = -\frac{e}{m_e} \vec{S}}$$

Combining all together :

note $\frac{1}{4\pi\epsilon_0}$ is gone! We moved to CGS units
 $\frac{e^2}{4\pi\epsilon_0} \rightarrow e^2$ Gaussian units

$$\hat{H}_1 = -\vec{\mu} \cdot \vec{B} = +\frac{1}{2} \frac{Ze^2}{m_e^2 c^2} \frac{1}{r^3} \hat{S} \hat{L}$$

Our perturbation due to Spin-Orbit coupling

Thomas precession since electron is accelerating (to move along orbit) and we cannot use it as inertial frame

So if we used only classical approach we would get the almost correct expression -

$$\frac{g}{2} = 1,001...$$

Time to think about states of electron.

so far we used $|n, l, m\rangle$

but we should include spin into consideration

$$|n, l, m\rangle \otimes |s, m_s\rangle$$

↑ analogous to l in

\hat{H}_0 has no clue about spin i.e. compute this way we ignored it.

We need to find good basis which states also eigen states of \hat{M}_z , or we have to deal with degenerate \hat{V} matrix. If we do it right \hat{V} will be diagonal and our life is "easy".

Let's look at total momentum operator $\hat{J} = \hat{L} + \hat{S}$

its eigen functions are constructed from

$$|l, m\rangle \otimes |s, m_s\rangle \rightarrow |j, l, s, m_j\rangle, \quad \begin{matrix} j = |l-s| \dots |l+s| \\ m_j = -j, \dots, 0, \dots, j \end{matrix}$$

so they are eigen functions of $\hat{M}_z, \hat{S}^2, \hat{L}^2, \hat{J}^2, \hat{J}_z$

Old $|s, m_s\rangle$
 $|l, m\rangle$
 are bad basis
 because \hat{S}, \hat{L}
 do not conserve
 $[\hat{M}_z, \hat{L}] \neq 0$
 $[\hat{M}_z, \hat{S}] \neq 0$

Note

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

$$\hat{L}\hat{S} = \frac{1}{2} (\hat{J}^2 - \hat{L}^2 - \hat{S}^2)$$

$$\hat{L}\hat{S} |j, l, s, m_j\rangle = \frac{1}{2} \hbar^2 (j(j+1) - l(l+1) - s(s+1))$$

"
 $\frac{1}{2}$ for electron

Reminder about angular momentum / spin addition

$$\hat{J} = + \left\{ \begin{array}{l} \hat{L} ; \hat{L}_z \rightarrow m_l \\ \hat{S} ; \hat{S}_z \rightarrow m_s \end{array} \right\} + \Rightarrow \begin{array}{l} \text{maximum } m = l + s \\ \text{minimum } m = |l - s| \end{array}$$

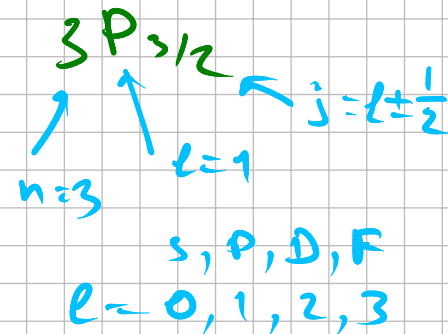
Think about vector addition

Generally speaking, there are multiple ways to get the same m_j out of different m_l, m_s so we expect such $|j, m_j\rangle$ to be superpositions of same l, s but different $m_l + m_s = m_j$

Wonderful properties

$$\begin{aligned} \hat{J}^2 |j, l, s, m_j\rangle &= \hbar^2 j(j+1) |j, l, s, m_j\rangle \\ \hat{L}^2 |j, l, s, m_j\rangle &= \hbar^2 l(l+1) |j, l, s, m_j\rangle \\ \hat{S}^2 |j, l, s, m_j\rangle &= \hbar^2 s(s+1) |j, l, s, m_j\rangle \\ \hat{J}_z |j, l, s, m_j\rangle &= \hbar m_j |j, l, s, m_j\rangle \end{aligned}$$

Spectroscopic level notation



$$\Rightarrow \hat{L}\hat{S}|j, l, s, m_j\rangle = \frac{1}{2} \hbar^2 \left(j(j+1) - l(l+1) - \frac{3}{4} \right) |j, l, s, m_j\rangle$$

$$j = l \pm \frac{1}{2}$$

electron spin

$$\langle n, j, l, s, m_j | \frac{\hat{L}\hat{S}}{r^3} | n, j, l, s, m_j \rangle =$$

note \uparrow same as $|n, l, m\rangle = |R_{nl}\rangle |Y_{lm}\rangle$

$$= \langle n, j, l, s, m_j | \frac{1}{r^3} | n, j, l, s, m_j \rangle \cdot \frac{1}{2} \hbar^2 \left(j(j+1) - l(l+1) - \frac{3}{4} \right)$$

this one is tricky

$$= \frac{Z^3}{l(l + \frac{1}{2})(l+1) n^3 a^3}$$

$$\begin{cases} (l + \frac{1}{2})(l + \frac{1}{2} + 1) - l(l+1) - \frac{3}{4} \\ (l - \frac{1}{2})(l - \frac{1}{2} + 1) - l(l+1) - \frac{3}{4} \\ \cancel{l^2} + \cancel{l} + \frac{1}{4} + \cancel{l} + \frac{1}{2} - \cancel{l^2} - \cancel{l} - \frac{3}{4} \\ \cancel{l^2} - \cancel{l} + \frac{1}{4} + \cancel{l} - \frac{1}{2} - \cancel{l^2} - \cancel{l} - \frac{3}{4} \\ \left. \begin{cases} l & , j = l + \frac{1}{2} \\ -(l+1) & , j = l - \frac{1}{2} \end{cases} \right\} \end{cases}$$

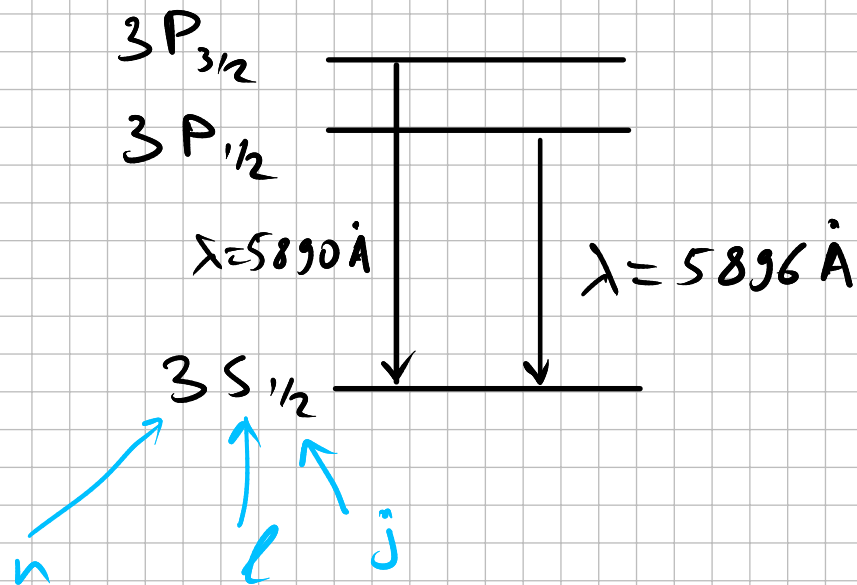
all together

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

spin orbit correction

Note $E_{s-o}^{(1)} = 0$ for $l=0$! since $\vec{L}=0$

Remember sodium doublet in physics 251?



It is interesting that $E_{s-o}^{(1)} \sim m_e c^2 \alpha^4$

HW: same as relativistic correction
so we need to add them together