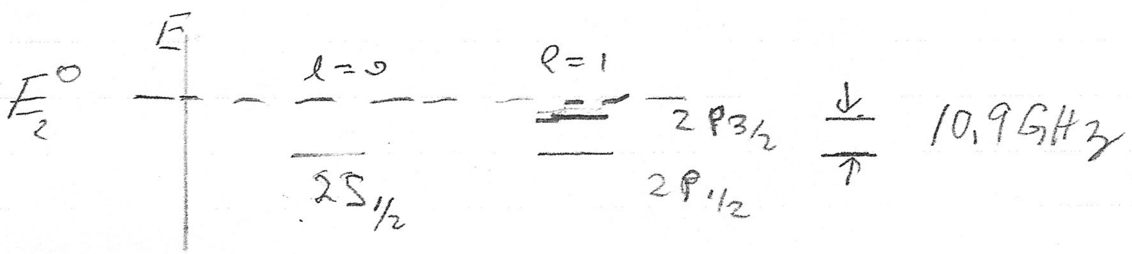
Phys 522

Fine Structure

Relativistic corrections $\mathcal{O}(\alpha^4)$



$\vec{J} = \vec{L} + \vec{S}$ rotational invariance $[\hat{H}, \hat{J}^2] = 0$

$E_{n,j}$ n, j good quantum numbers

$\Delta E\,(2S - 1S) = 10.2\,eV$

$\Delta E\,(10\,GHz) = 10^{10}(2\pi)(6.58\times 10^{-16}\,eV\cdot s) = 4.1\times 10^{-5}\,eV$
$\hbar$

$\alpha^{-2} \simeq 20{,}000\ (18769)$

Exact solution from Dirac equation (Gordon, 1928)

$$E_{n,j} = mc^2\left[1 + \left(\frac{Z\alpha}{n - (j+\frac{1}{2}) + \sqrt{(j+\frac{1}{2})^2 - (Z\alpha)^2}}\right)^2\right]^{-1/2}$$

Expect relativistic corrections to be small

$\langle K \rangle = \langle H \rangle - \langle V \rangle$, $\langle V \rangle = -e^2\left\langle \frac{1}{r}\right\rangle = \frac{-e^2}{a_0 n^2} = 2E_n^0$

$\langle K \rangle = \frac{1}{2}\frac{mc^2\alpha^2}{n^2} \ll mc^2$

speed

$\langle K \rangle_{ground} = \frac{1}{2}m(c\alpha)^2 = \frac{1}{2}m\langle v^2\rangle \Rightarrow \sqrt{\langle v^2\rangle} = c\alpha$

Expand exact solution:

$$E_{nj} \cong mc^2 \left\{ 1 - \frac{1}{2}\frac{(Z\alpha)^2}{n^2}\left[1 + \frac{(Z\alpha)^2}{n}\left(\frac{1}{j+1/2} - \frac{3}{4n}\right)\right]\right\}$$

$$\hat{H} \cong mc^2 + \frac{p^2}{2m} \underbrace{- \frac{p^4}{8m^3c^2}}_{\substack{H_K \\ \text{kinetic}}} \underbrace{+ \frac{e}{2mc}\vec{S}\cdot\vec{B}'}_{\substack{H_{SO} \\ \text{spin orbit}}} \underbrace{+ \frac{\hbar^2}{8m^2c^2}\nabla^2 V}_{\substack{H_D \\ \text{Darwin}}}$$

$\vec{B}'$ is internal magnetic field due to motion of electron around proton

In external magnetic field (Zeeman effect)

$$\hat{H}_{ext} = -\vec{\mu}\cdot\vec{B} = \frac{e}{2mc}\left(\vec{L} + \underset{\overset{\shortparallel}{2}}{g}\vec{S}\right)\cdot\vec{B}$$

Kinetic energy correction

$$K = \left[(pc)^2 + (mc^2)^2\right]^{1/2} - mc^2$$

$$\cong mc^2\left[1 + \frac{1}{2}\left(\frac{pc}{mc^2}\right)^2 - \frac{1}{8}\left(\frac{pc}{mc^2}\right)^4\right] - mc^2$$

$$= \frac{1}{2}\frac{p^2}{2m} - \frac{1}{8}\frac{p^4}{m^3c^2}$$

Since $[H_k, L^2] = 0$, kinetic correction does not mix states of different ℓ, m

First order perturbative correction

$$E^{(1)}_{n\ell} = -\langle n\ell m | \frac{1}{8}\frac{p^4}{m^3c^2} | n\ell m\rangle$$

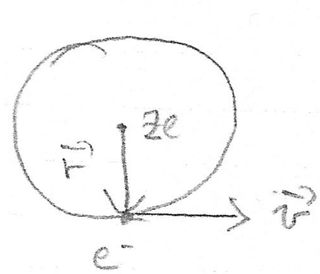
$$= -\frac{\alpha^4 mc^2}{2}\left[-\frac{3}{4n^4} + \frac{1}{n^3}\frac{1}{(\ell+\frac{1}{2})}\right]$$

Spin-Orbit

effective $\vec{B}'$ due to orbital motion $\frac{1}{\ell}$ generates magnetic field in rest frame of electron.

Classically:

nucleur rest frame



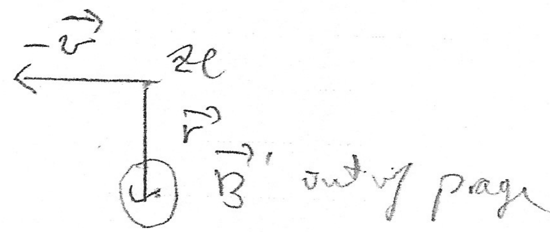
$\vec{L} = m\vec{r}\times\vec{v}$ out of page

$\vec{\mathcal{E}} = \frac{Ze\vec{r}}{r^3}$

In electron rest frame:

$$\vec{B}' = \left(-\frac{\vec{v}}{c}\right)\times\vec{\mathcal{E}} = \frac{-Ze}{r^3}\left(\frac{\vec{v}}{c}\right)\times\vec{r} = \frac{Ze}{mcr^3}\vec{L}$$

e^- rest frame

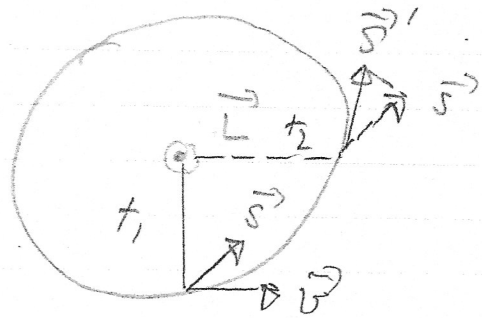


Torque on electron in electron rest frame

$$\left(\frac{d\vec{S}}{dt}\right)_{\substack{e^- \\ rest}} = \vec{\mu} \times \vec{B}' = \left(\frac{-ge}{2mc}\right)\vec{S} \wedge \left(\frac{Ze}{mcr^3}\right)\vec{L}$$

$$= \frac{-Ze^2 g}{2m^2c^2r^3}\left(\vec{S}\times\vec{L}\right) \quad \text{where } g=2 \text{ from Dirac}$$

Projection of $\vec{S}$ onto orbital plane precesses counter clockwise,



proton rest frame

Corresponding energy,

$$\vec{H} = -\vec{\mu}\cdot\vec{B}' = \frac{ge}{2mc}\,\vec{S}\cdot\vec{B}'$$

with $g=2$, this is twice as large as

term in expansion of Dirac energy. The error, first pointed out by Thomas is known as the Thomas precession. The effect is due to transformation between rotating frame of reference.

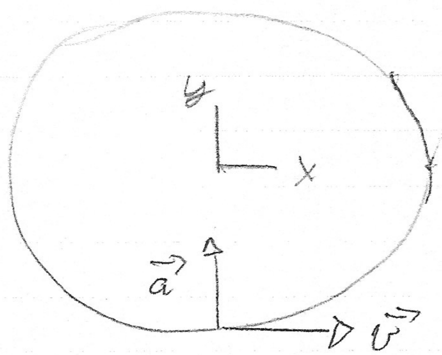
Thomas Precession ($\vec{\omega}_T$) (1927)

$$\left(\frac{d\vec{S}}{dt}\right)_{\text{nuclear}} = \left(\frac{d\vec{S}}{dt}\right)_{\substack{e^- \\ \text{rest}}} + \vec{\omega}_T \times \vec{S}$$

In special relativity, combination of Lorentz boosts in different directions is equivalent to (boost) × (rotation), general Lorentz transformation.

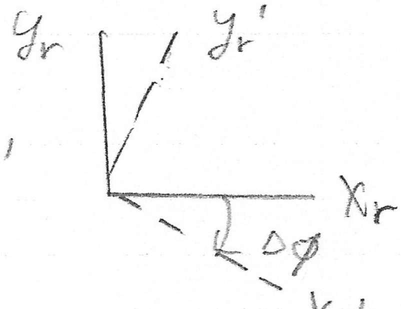
Simple explaination from Taylor + Wheeler *Spacetime Physics*

Consider rotating frame with acceleration $\vec{a}$.
x-y denotes fixed inertial frame



rotating frame precesses clockwise by $\Delta\phi$ per rotation

after one rotation,



$$\Delta\phi = \pi\left(\frac{v}{c}\right)^2$$

$$|\vec{\omega}_T| = \Delta\phi\left(\frac{v}{2\pi r}\right) = \frac{v^2}{c^2}\left(\frac{v}{2r}\right) = \frac{1}{2}\frac{v}{c^2}a$$

giving $\quad \vec{\omega}_T = -\frac{1}{2c^2}\vec{v}\times\vec{a}$

Acceleration of e^- in atom due to nuclear electric field,

$$\vec{a} = -\frac{e}{m}\vec{\mathcal{E}} = \frac{-Ze^2}{mr^3}\vec{r}$$

$$\vec{\omega}_T = \left(-\frac{1}{2c^2}\right)\vec{v} \times \left(-\frac{Ze^2}{mr^3}\vec{r}\right) = \frac{-e}{2mc}\vec{B}' \propto -\vec{L}$$

term $\quad \vec{\omega}_T \times \vec{S} = \left(\frac{-Ze^2}{2mc^2r^3}\vec{L}\right) \times \vec{S} = \frac{+Ze^2}{2m^2r^3}\vec{S}\times\vec{L}$

then correct torque is

$$\left(\frac{d\vec{S}}{dt}\right)_{nuclear} = \frac{-Ze^2}{2m^2c^2r^3}\left(\underbrace{g\,\vec{S}\times\vec{L} - \vec{S}\times\vec{L}}_{(g-1)\,\vec{S}\times\vec{L} = \vec{S}\times\vec{L}}\right)$$

Then we get $\frac{1}{2}$ previous,

$$H_{so} = \frac{Ze^2}{2m^2c^2r^3}\left(\vec{L}\cdot\vec{S}\right) = \frac{e}{2mc}\vec{S}\cdot\vec{B}'$$

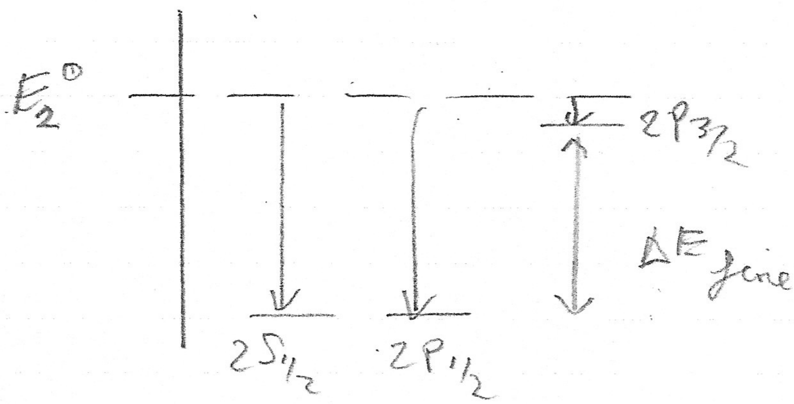
$$= \frac{1}{4}(Z\alpha)^4 mc^2\left(\frac{a_0}{Zr}\right)^3 \frac{2\,\vec{L}\cdot\vec{S}}{\hbar^2}$$

shows α^4 dependence

<u>Finally, Darwin</u> term effects only $l=0$ state and is

$$E_{D,n,0} = \frac{1}{2n^3}mc^2(Z\alpha)^4$$

Combing all correction we find
result depends only on j.



$$n=2 \qquad \Delta E_{fine} = \frac{4}{128}\, mc^2 (Z\alpha)^4$$

$$\Delta f_{fine} = \frac{\Delta E_{fine}}{h} = 10.9\ \text{GHz}$$

Test of theory is degeneracy of $2S_{1/2}$, $2P_{1/2}$.

Split by Lamb shift $\Delta f_L = 1{,}057\ \text{GHz}$