Fine Structure

Note Title

12/28/2004

Fine structure comes from relativistic corrections to electronic wavefunctions

→ Think of fine structure correction as Dirac eqn. − Schrodinger eqn

Use the Pauli equation as a starting point (approximation to Dirac equation to lowest order in v/c)

$$H = \underbrace{mc^2}_{\text{rest energy}} + \underbrace{p^2/2m - \frac{Ze^2}{4\pi\varepsilon_0 r}}_{\text{non-relativistic}} + \underbrace{H_{FS}}_{\text{fine structure}}$$

$$H_{FS} = \underbrace{\frac{-p^4}{8m^3c^2}}_{\text{kinetic}} + \underbrace{\frac{\hbar^2}{2m^2c^2}\frac{1}{r}\frac{\partial V}{\partial r}\vec{L}\cdot\vec{S}}_{\text{spin-orbit}} + \underbrace{\frac{\pi\hbar^2}{2m^2c^2}\frac{Ze^2}{4\pi\varepsilon_0}\delta(\vec{r})}_{\text{"Darwin"}}$$

Kinetic: relativistic correction to kinetic energy

$$E = \sqrt{(mc^2)^2 + (pc)^2}$$

$$KE = E - mc^2 = mc^2\left(\sqrt{1 + p^2/m^2c^2} - 1\right) \simeq mc^2\left(1 + \frac{1}{2}\frac{p^2}{m^2c^2} - \frac{1}{8}\frac{p^4}{m^4c^4} - 1\right)$$

with $p^2 \ll m^2c^2$

$$KE = \underbrace{\frac{p^2}{2m}}_{\text{regular kinetic energy}} - \underbrace{\frac{1}{8}\frac{p^4}{m^3c^2}}_{\text{correction}}$$

Spin-orbit :

interaction of electron magnetic moment with motional magnetic field (relativistic $\vec{v}\times\vec{E}$, where $\vec{E}$ is from the nucleus)

only for Hydrogenic atoms

$$\vec{B} = -\frac{\vec{v}\times\vec{E}}{c^2} = -\frac{\vec{v}}{c^2}\times(-\vec{\nabla}V) = \frac{\vec{v}}{c^2}\,\vec{\nabla}\left(\frac{Ze}{4\pi\varepsilon_0 r}\right)$$

$$= \frac{\vec{v}}{c^2}\times\frac{\vec{r}}{r}\left(\frac{-Ze}{4\pi\varepsilon_0 r^2}\right) = \frac{Ze\hbar}{4\pi\varepsilon_0 m c^2 r^3}\,\vec{L} \quad \left(\text{since: } \hbar\vec{L} = m\vec{r}\times\vec{v}\right)$$

interaction energy $= -\vec{\mu}\cdot\vec{B}$ where

from Dirac theory

$$\vec{\mu} = -g\frac{e\hbar}{2m}\vec{S} \quad \text{and} \quad g \simeq 2 \quad (\text{for an electron})$$

QED – $g \neq 2$

* $\mu_0 = 1.4\ \text{MHz/gauss} \times h = \frac{e\hbar}{2m}$ Bohr magneton

Many AMO experimentalists like frequencies as units

There is another contribution to the interaction energy from Thomas precession (see Jackson)

- relativistic transformation of vector between frames involves a rotation if the relative accelerations are non-colinear
- observer fixed at the nucleus sees this as an additional magnetic field

Thomas precession cuts the energy in half, so

$$H_{LS} = -\vec{\mu}\cdot\vec{B} = \frac{1}{4\pi\varepsilon_0}\frac{Ze^2\hbar^2}{m^2c^2r^3}\vec{L}\cdot\vec{S}\left(\frac{1}{2}\right)$$

More generally: $H_{LS} = \frac{1}{2}\frac{\hbar^2}{m^2c^2}\vec{L}\cdot\vec{S}\,\frac{1}{r}\frac{\partial V}{\partial r}$ — we'll see soon why this may not be $1/r^2$

With $\vec{J} = \vec{L} + \vec{S}$, $\vec{L}\cdot\vec{S} = \frac{1}{2}(J^2 - L^2 - S^2)$

(remember the triangle inequality! $j = l+s \ldots l-s$)

$$\Rightarrow \frac{\hbar^2}{2}\underbrace{\left[j(j+1) - l(l+1) - s(s+1)\right]}_{\text{vanishes if } l=0\,!}$$

So, to first order in perturbation theory:

$$\Delta E_{LS} = \frac{1}{2mc^2}\frac{Ze^2\hbar^2}{4\pi\varepsilon_0}\left\langle\frac{1}{r^3}\right\rangle\left[j(j+1) - l(l+1) - s(s+1)\right]$$

*just for Hydrogenic atoms

Darwin term:

hard to understand "Zitterbewegung" – electrons jitter on a length scale $\hbar/mc \sim 400$ fm

So, the electron experiences the electric potential averaged over this length scale – getting this calculation right is very hard

$$H_D = \frac{\pi\hbar^2 Ze^2}{2m^2c^2}\frac{1}{4\pi\varepsilon_0}\delta(\vec{r}) \qquad \langle H_D\rangle \neq 0 \text{ for } l=0 \text{ only!}$$

Overall: everything is diagonal in $\vec{J}$ basis

$$\Delta E = \langle nlj | H_{KE} + H_{LS} + H_D | nlj\rangle \quad \text{use } 1^{st} \text{ order P.T.}$$

Adding everything up: $E_{nj} = E_n\left[1 + \frac{(Z\alpha)^2}{n^2}\left(\frac{n}{j+1/2} - 3/4\right)\right]$

agree to order $(Z\alpha)^2$

(surprise – no l dependence)

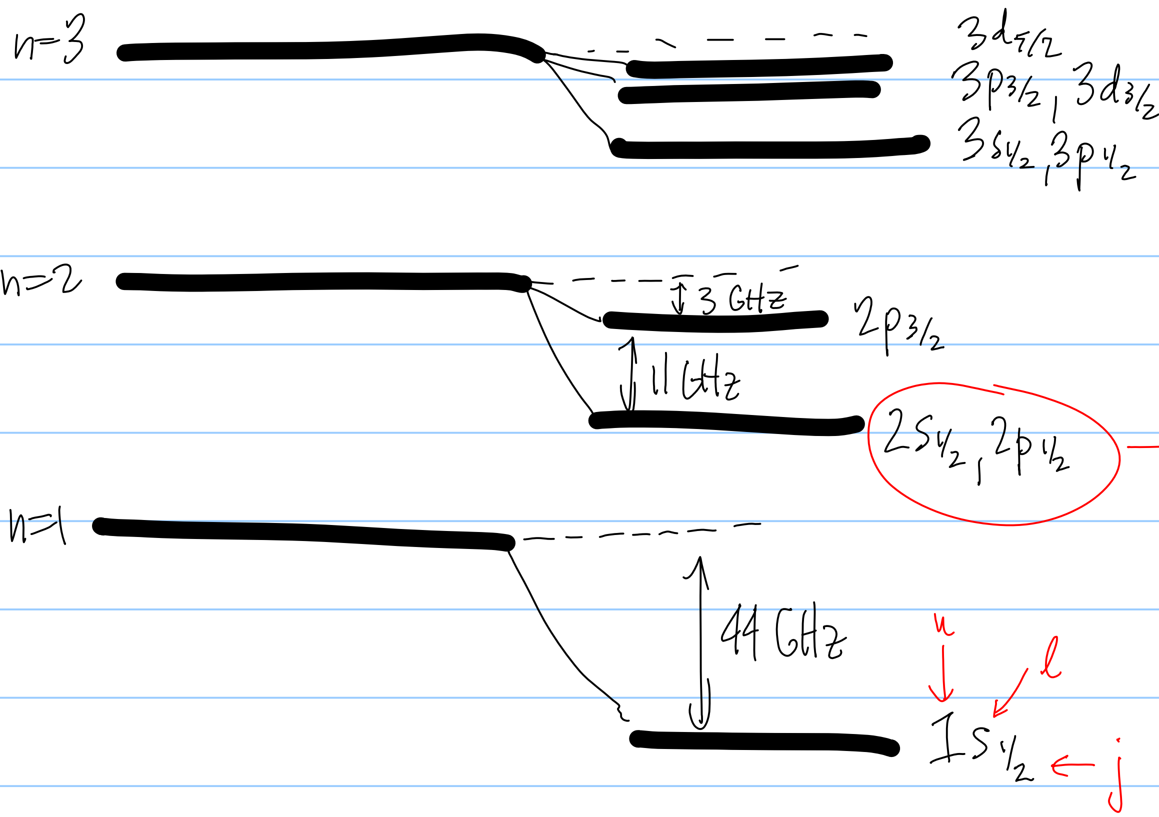
fine structure constant – correction to energy $\sim \alpha^2$

Exact result from Dirac equation:

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

(both equations are for Hydrogen-like atoms only)

What does Hydrogen look like?



— states with the same n, l are degenerate — Lamb shift removes this degeneracy

- in Hydrogen, all three terms contribute about equally
- in alkalis, mostly spin-orbit