Lecture 16

Finish up spin-orbit coupling & fine structure

Last time got spin-orbit perturbation

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

Can sort of see where it comes from, to within a few factors of 2

Want to evaluate in perturbation theory

Since H' is rotationally invariant, expect eigenstates of $\vec{J} = \vec{L} + \vec{S}$ to be good

Write

$$|n\,l\,s\,j\,m_j\rangle = \sum_{m_l, m_s} C^{l\ s\ j}_{m_l\ m_s\ m_j} |n\,l\,m_l\,s\,m_s\rangle$$

↑ Clebsch-Gordan coeffs

But if we only care about energy shifts, don't need state relations...

Use

$$E^{(1)} = \langle n l s j m_j | H' | n l s j m_j \rangle$$

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

So

$$E^{(1)} = \frac{1}{2} \frac{e^2}{4\pi\varepsilon_0} \frac{1}{m^2c^2} \left\{ \frac{\hbar^2}{2} \left[j(j+1) - l(l+1) - \underbrace{s(s+1)}_{\frac{1}{2}\cdot\frac{3}{2} = \frac{3}{4}} \right] \right\} \left\langle \frac{1}{r^3} \right\rangle$$

Do need $\langle \frac{1}{r^3} \rangle$, independent of spin, so just an integral

Again, need to evaluate using tricks, see in HW

Find $\langle \frac{1}{r^3} \rangle = \frac{1}{l(l+\frac{1}{2})(l+1)} \frac{1}{n^3 a^3}$

Gives

$$E^{(1)} = \frac{1}{4} \frac{e^2}{4\pi\varepsilon_0} \frac{\hbar^2}{m^2c^2} \frac{1}{n^3a^3} \left[\frac{j(j+1) - l(l+1) - \frac{3}{4}}{l(l+\frac{1}{2})(l+1)} \right]$$

Use $\frac{e^2}{4\pi\varepsilon_0} = -2aE_1$

(recall $E_1 = E_1^{(0)}$ = unperturbed ground state energy -13.6 eV)

and $\frac{\hbar^2}{ma^2} = -2E_1$

Get

$$E^{(1)} = \frac{E_1^2}{mc^2} \frac{1}{n^3} \left[\frac{j(j+1) - l(l+1) - \frac{3}{4}}{l(l+\frac{1}{2})(l+1)} \right]$$

See that $\frac{\Delta E}{E} \sim \frac{E}{mc^2}$, same as for relativistic correction

Maybe surprising, but makes sense:

- Had to wave hands about several relativistic effects in derivation of H'

(g-factor, Thomas precession)

- Magnetism is inherently relativistic
  comes from moving charges

So in fact, spin-orbit effect has same magnitude as relativistic effect, makes sense to combine them.

(Note, H'_{rel} is still diagonal in $|j\,m_j\rangle$ basis)

Problem 6.17: Mehdi Kabir

$$\Rightarrow E_n^{(1)} = \frac{E_1^2}{2mc^2}\,\frac{1}{n^4}\left(3 - \frac{4n}{j+\frac{1}{2}}\right)$$

Maybe a little surprising.

Usually when a bunch of unrelated, complicated effects add up to something simple, means there is something more going on

And there is:
Recall Dirac eqn = relativistic version of Schr Eqn

Can be solved exactly for Coulomb potential

Find

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

where α = fine structure constant

$$\alpha^2 = -\frac{2E_1}{mc^2} \approx \left(\frac{1}{137}\right)^2$$

Taylor expand for small α:

$$E_{nj} \approx mc^2 \left[1 - \frac{\alpha^2}{2n^2} + \frac{1}{8}\frac{\alpha^4}{n^4}\left(3 - \frac{4n}{j+\frac{1}{2}}\right) + \dots \right]$$

$$\underbrace{1}_{\text{rest energy}} \qquad \underbrace{- \frac{\alpha^2}{2n^2}}_{\text{Bohr energy}} \qquad \underbrace{+ \frac{1}{8}\frac{\alpha^4}{n^4}\left(3 - \frac{4n}{j+\frac{1}{2}}\right)}_{\text{fine structure.}}$$

So really, relativistic correction and spin-orbit effect are two parts of the same thing.

About solution:

Recall we saw that relativistic correction broke degeneracy in l:
2s + 2p states had different shift

See that total effect lifts degeneracy in j

Ground state: $l = 0$, so $j = s = \frac{1}{2}$ $\quad m_j = m_s$

No degeneracy to lift, level just shifted by

$$E^{(1)}_{1\frac{1}{2}} = \frac{E_1^2}{2mc^2}\left(3 - \frac{4}{1}\right) = -\frac{E_1^2}{2mc^2}$$

$$= -\frac{(13.6\,\text{eV})^2}{2\cdot(511\,\text{keV})}$$

$$= -1.8\times10^{-4}\,\text{eV}$$

$$= h \times 43.7\,\text{GHz}$$

In first excited state, have 8 states all together:

In j basis:

	n	ℓ	s	j	m	
$\vert$	2	0	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\rangle$
$\vert$	2	0	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\rangle$
$\vert$	2	1	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\rangle$
$\vert$	2	1	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\rangle$
$\vert$	2	1	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{3}{2}$	$\rangle$
$\vert$	2	1	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$\rangle$
$\vert$	2	1	$\frac{1}{2}$	$\frac{3}{2}$	$-\frac{1}{2}$	$\rangle$
$\vert$	2	1	$\frac{1}{2}$	$\frac{3}{2}$	$-\frac{3}{2}$	$\rangle$

All four $j=\frac{1}{2}$ states have same energy

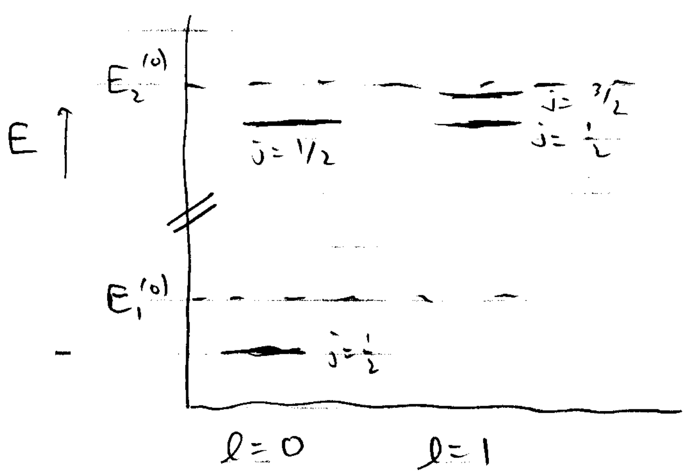
$$E^{(1)}_{2\,\frac{1}{2}} = \frac{E_1^2}{2mc^2}\,\frac{1}{2^4}\left(3-\frac{8}{1}\right) = -\frac{5}{32}\,\frac{E_1^2}{mc^2}$$

and four $j=\frac{3}{2}$ state have another

$$E^{(1)}_{2\,\frac{3}{2}} = \frac{E_1^2}{2mc^2}\,\frac{1}{2^4}\left(3-\frac{8}{2}\right) = -\frac{1}{32}\,\frac{E_1^2}{mc^2}$$

(note shift always negative)

Picture:



Recall atomic state notation

$^2P_{3/2} \to J$

see why it is needed