

Hydrogen + Fine Structure

aka Relativistic Perturbations

Review: (unperturbed)

$$E_n = - \left[\frac{m}{2\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0} \right)^2 \right] \frac{1}{n^2} \quad \begin{array}{l} \ell: \text{from } 0 \text{ to } n-1 \\ \text{NO DEPENDENCE} \\ \text{ON } \ell \text{ in } E_n \end{array}$$

p. 149, eq 4.70 $n=1, 2, \dots, \infty$

Another way to write this (important)

$$E_n = - \frac{1}{2} \left(\frac{e^2}{4\pi\epsilon_0 \hbar c} \right)^2 mc^2 \times \frac{1}{n^2}$$

fine structure constant $\alpha \approx 1/137$

$$E_n = - \frac{1}{2} \alpha^2 mc^2 \times \frac{1}{n^2} \quad \begin{array}{l} \text{technically} \\ m = \frac{m_e m_p}{m_e + m_p} \end{array}$$

Think of $\frac{v_e}{c} = \frac{\alpha}{nc}, E_n \approx -\frac{1}{2} m v_e^2$

Actually, virial theorem, p. 190 Eq 4.191

$$\langle T \rangle = -E_n = +\frac{1}{2} m v_e^2$$

$$\langle V \rangle = 2E_n \quad \text{now note ...}$$

$$2E_n = - \frac{e^2}{4\pi\epsilon_0} \cdot \frac{1}{\frac{4\pi\epsilon_0 \hbar^2}{m_e^2}} \cdot \frac{1}{n^2}$$

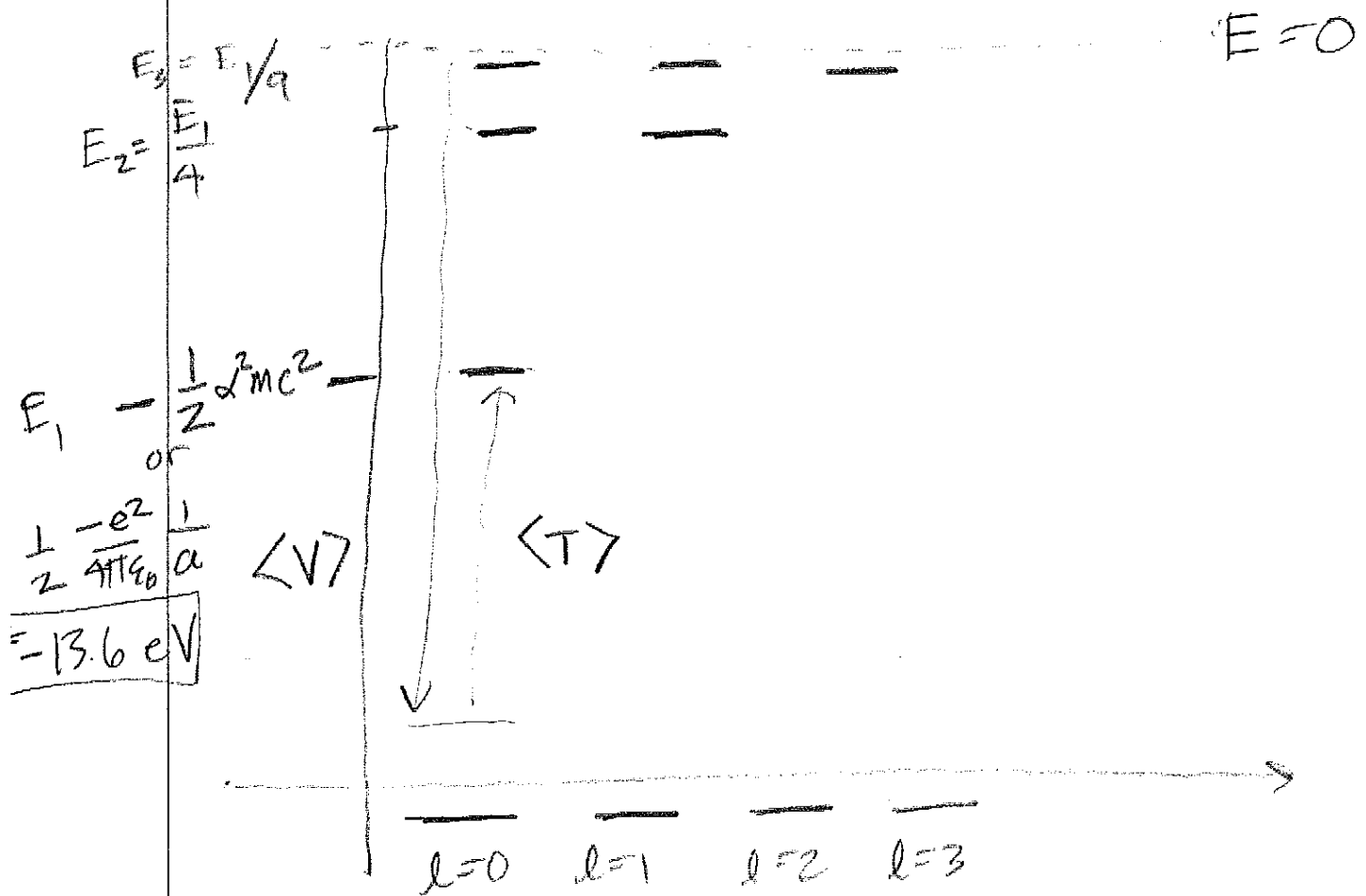
Bohr radius a

note:

$$a = \frac{1}{\alpha} \cdot \frac{\hbar}{m_e c} = \frac{4\pi\epsilon_0 \hbar^2}{e^2 m_e}$$

$$2E_n = - \frac{e^2}{4\pi\epsilon_0} \cdot \frac{1}{a} \cdot \frac{1}{n^2}$$

For $-\frac{e^2}{4\pi\epsilon_0 r}$ potential



Relativistic Corrections

Griffiths. always m

$$O\left(\frac{E_n^2}{m c^2}\right) \Rightarrow O\left(\frac{m^2 v_e^4}{m c^2 n^4}\right) \Rightarrow O\left[\left(\frac{v_e}{nc}\right)^4 \cdot m_e c^2\right]$$

$$O\left[\left(\frac{1}{137}\right)^2 \cdot 13.6\right]$$

$$\sim 5 \cdot 10^{-5} \times 13.6 \sim 7 \cdot 10^{-4} \text{ eV}$$

"resolution" needed

$$\text{or, } \lambda = \frac{2\pi\hbar c}{E} \sim \frac{2\pi \cdot 197.3 \text{ eV} \cdot \text{nm}}{7 \cdot 10^{-4}} \sim 1.8 \text{ nm}$$

More specifically, the precise prefactor needed is:

$$\frac{2(E_n^2)}{mc^2} = \frac{2 \cdot \frac{1}{4} \alpha^4 mc^4}{mc^2 n^4} = \frac{\alpha^2}{n^2} \left[\frac{1}{2} \frac{\alpha^2 mc^2}{n^2} \right]$$

$$= \frac{\alpha^2}{n^2} |E_n| \quad \underbrace{\hspace{10em}}_{E_r'(n, l)}$$

$$(A) H_r' = -\frac{P^4}{8m^3c^2} \Rightarrow E_r' = \alpha^2 |E_n| \left[-\frac{1}{n^2} \left[\frac{n}{l+\frac{1}{2}} - \frac{3}{4} \right] \right]$$

$E_r'(n, l)$

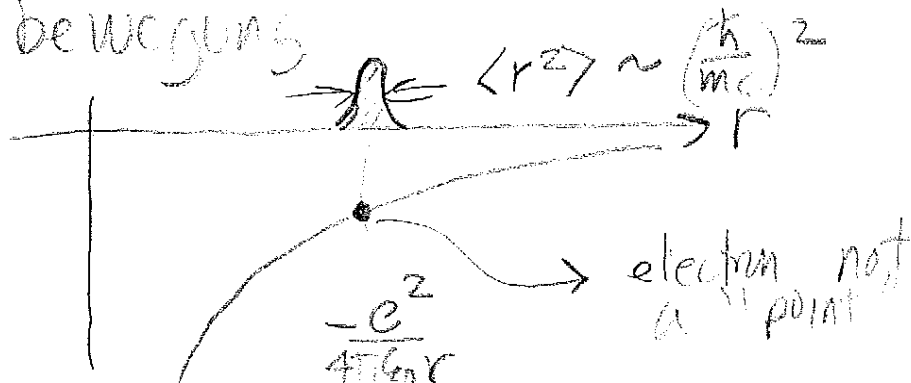
$n=5$	-0.370	-0.103	-0.050	-0.0271	-0.0144
$n=4$	-0.453	-0.120	-0.053	-0.0246	X
$n=3$	-0.583	-0.139	-0.050	X	X
$n=2$	-0.813	-0.146	X	X	X
$n=1$	-1.25	X	X	X	X
	$l=0$	$l=1$	$l=2$	$l=3$	$l=4$

↑ slower

→ slower

(B) Neglected in text... the "Darwin" Term... physics is the electron is "spread out" over a distance of $\lambda \sim \frac{\hbar}{mc}$

"Zitterbewegung"



Darwin Term Discussion

Note (p. 270, Eq. 6.57) the $\alpha(p^4)$ shift is...

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

when $l=0$ (s-wave)

$$E_r^1 = -\frac{1}{2} \frac{(E_n^2)}{mc^2} [8n - 3] \quad (\alpha)$$

now, compare with (p. 274, Eq. 6.66), the complete $O\left(\frac{E_n^2}{mc^2}\right)$ shift:

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

superficially, resembles Eq. 6.57, with l replaced by j . This is a big deal, though. when $l=0$, $j=s=\frac{1}{2}$ (spin of electron).

Now...

$$E_{fs}^1 = -\frac{1}{2} \frac{E_n^2}{mc^2} [4n - 3] \quad (\beta)$$

Main point: This difference between (α) and (β) cannot be due to the spin-orbit interaction, because $l=0$ so $\langle \vec{L} \cdot \vec{S} \rangle = 0$. The difference between (α) & (β) is caused by yet another physical effect, "The Darwin Term".

Physics underlying the Darwin Term...

the electron is "smeared out" over a distance scale of approximately its Compton Wavelength (reduced).

Compton Wavelength $\equiv \frac{\hbar}{mc} \equiv \lambda$
 (reduced)

note: $\lambda = \frac{\hbar}{mc} = \frac{e^2}{4\pi\epsilon_0 \hbar c} \cdot \frac{\hbar^2}{me^2} \cdot 4\pi\epsilon_0$

fine structure constant α
 p. 267 Eq 6.43

Bohr Radius a
 p. 150 Eq 4.72

$\lambda = \alpha a \quad \alpha \approx \frac{1}{137}$

Because the electron is spread out, it doesn't quite feel the $1/r$ potential... instead...

$\langle V_{\text{eff}}(\vec{r}) \rangle \approx -\frac{e^2}{4\pi\epsilon_0 r} + \frac{1}{2} \left(\langle x^2 \frac{\partial^2 V}{\partial x^2} \rangle + \langle y^2 \frac{\partial^2 V}{\partial y^2} \rangle + \langle z^2 \frac{\partial^2 V}{\partial z^2} \rangle \right)$

↑ averaged over electron spread

point particle

- no linear term - no net \vec{E} field or "direction" to electron blob.
- no direction special...

$\rightarrow \langle x^2 \frac{\partial^2 V}{\partial x^2} \rangle + \langle y^2 \frac{\partial^2 V}{\partial y^2} \rangle + \langle z^2 \frac{\partial^2 V}{\partial z^2} \rangle$

$\approx \frac{1}{3} \langle r^2 \rangle \langle \nabla^2 V \rangle$ poisson equation

-- $\frac{e p(\vec{r})}{\epsilon_0}$ $p(\vec{r}) = e \delta(\vec{r})$ proton

so

$\langle V_e(\vec{r}) \rangle \approx -\frac{e^2}{4\pi\epsilon_0 r} + \frac{e^2 \langle r^2 \rangle \delta(\vec{r})}{6\epsilon_0}$

Darwin Term

$= \lambda^2 = \alpha^2 a^2$

only influences when electron sits on proton

The perturbation introduced by the Darwin term only influences $l=0$ states, because they are the only ones where the electron sits on the position. The electron energy gets pushed up. By how much (approximately)?

$$\langle H_{\text{Darwin}} \rangle = \frac{e^2}{6\epsilon_0} \alpha^2 a^2 \langle \psi_{n00} | \delta(\vec{r}) | \psi_{n00} \rangle$$

$$= |\psi_{n00}(0)|^2$$

p. 151, Eq. 4.80

$$|\psi_{n00}(0)|^2 = \frac{1}{\pi a^3 n^3}$$

$a \rightarrow a \cdot n$
(p. 150, Eq. 4.73)

$$\langle H_D \rangle = \frac{1}{6} \alpha^2 \frac{e^2}{4\pi\epsilon_0 a} \frac{1}{n^4} \cdot 4n$$

($l=0$ only).

note:

$$\frac{E_n^2}{mc^2} = \frac{m^2}{4h^4} \left(\frac{e^2}{4\pi\epsilon_0} \right)^4 \frac{1}{n^4} \frac{1}{mc^2}$$

p. 149, Eq. 4.70

$$= \frac{1}{4} \left(\frac{e^2}{4\pi\epsilon_0 hc} \right)^2 \cdot \left(\frac{e^2}{4\pi\epsilon_0} \right) \left(\frac{me^2}{h^2 4\pi\epsilon_0} \right) \frac{1}{n^4}$$

$$\frac{1}{a}$$

$$\frac{E_n^2}{mc^2} = \frac{1}{4} \alpha^2 \frac{e^2}{4\pi\epsilon_0 a} \frac{1}{n^4}$$

go back and compare with the difference between (a) + (b), which is

$$+ \frac{1}{2} \frac{E_n^2}{mc^2} \cdot 4n = \frac{1}{8} \alpha^2 \frac{e^2}{4\pi\epsilon_0 a} \frac{1}{n^4} \cdot 4n$$

Compare, "almost same"

After 3 pages of work --

$$E_D' = \alpha^2 |E_n| \left[\underbrace{+\frac{1}{n^2} \cdot n}_{\varepsilon_D'(n,0)} \right] \quad \text{when } l=0$$

$$= 0 \quad \varepsilon_D'(n,0) \quad l > 0$$

Add this to the table!

$\varepsilon_D'(n,l)$

$n=5$	-0.170	-0.103	-0.050	-0.0271	-0.0144	
$n=4$	-0.203	-0.120	-0.053	-0.0216		
$n=3$	-0.250	-0.139	-0.050			
$n=2$	-0.313	-0.146				
$n=1$	-0.250					
	$l=0$	$l=1$	$l=2$	$l=3$	$l=4$	

revised →

$$\varepsilon_{nd} = \varepsilon_r'(n,0) + \varepsilon_D'(n,0) = \left[-\frac{1}{n^2} \left[n - \frac{3}{4} \right] \right] \quad l=0$$

$$= \varepsilon_c'(n,l) = \left[-\frac{1}{n^2} \left[\frac{n}{l+\frac{1}{2}} - \frac{3}{4} \right] \right] \quad l > 0$$

(c) Spin-Orbit.

$$E_{so}^1 = 0 \quad l=0$$

$$= \frac{\alpha^2}{n^2} |E_n| \left(\frac{n [j(j+1) - l(l+1) - 3/4]}{2l(l+1/2)(l+1)} \right)$$

Two cases :

(i) $j_- = l - \frac{1}{2}$ or $l = j_- + \frac{1}{2}$

$$\text{then } E'_{s_{0-}} = \frac{\alpha^2 |E_n|}{n^2} \left(\frac{n [j_- (j_- + 1) - (j_- + \frac{1}{2})(j_- + \frac{3}{2}) - \frac{3}{4}]}{2(j_- + \frac{1}{2})(j_- + 1)(j_- + \frac{3}{2})} \right)$$

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

$$= \frac{\alpha^2 |E_n|}{n^2} \left(\frac{n(-j_- - \frac{3}{2})}{2(j_- + \frac{1}{2})(j_- + 1)(j_- + \frac{3}{2})} \right)$$

$$E'_{s_{0-}} = -\frac{\alpha^2 |E_n|}{n^2} \left(\frac{n}{(2j_- + 1)(j_- + 1)} \right) \quad (j_- = l - \frac{1}{2})$$

(ii) $j_+ = l + \frac{1}{2}$ or $l = j_+ - \frac{1}{2}$

$$E'_{s_{0+}} = \frac{\alpha^2 |E_n|}{n^2} \left(\frac{n [j_+ (j_+ + 1) - (j_+ - \frac{1}{2})(j_+ + \frac{1}{2}) - \frac{3}{4}]}{2(j_+ - \frac{1}{2}) j_+ (j_+ + \frac{1}{2})} \right)$$

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

$$= \frac{\alpha^2 |E_n|}{n^2} \left(\frac{n [j_+ - \frac{1}{2}]}{2(j_+ - \frac{1}{2}) j_+ (j_+ + \frac{1}{2})} \right)$$

$$E'_{s_{0+}} = +\frac{\alpha^2 |E_n|}{n^2} \left(\frac{n}{(2j_+ + 1) j_+} \right) \quad (j_+ = l + \frac{1}{2})$$

Note: $(2j_- + 1) E'_{s_{0-}} + (2j_+ + 1) E'_{s_{0+}} = 0$

"center of gravity" unchanged. since $j_+ = j_- + 1$

Now include, $l > 0$

$$E_{so}^1(n, j_-) = - \left(\frac{1}{n} \frac{1}{(2j_- + 1)(j_- + 1)} \right) \quad j_- = l - \frac{1}{2}$$

$$E_{tot}^1(n, l, j_-) = E_r^1(n, l) + E_{so}^1(n, j_-)$$

$$E_{so}^1(n, j_+) = + \left(\frac{1}{n} \frac{1}{(2j_+ + 1)j_+} \right)$$

$$E_{tot}^1(n, l, j_+) = E_r^1(n, l) + E_{so}^1(n, j_+)$$

Put this in a table, with care to split the $l > 0$ entries into two, j_- & j_+ :

	j_-	j_+	j_-	j_+	j_-	j_+	j_-	j_+
$n=5$	-0.170 $1/2$	-0.070 $3/2$	-0.0367 $5/2$	-0.020 $7/2$	-0.010 $9/2$			
		-0.170 $1/2$	-0.070 $3/2$	-0.0367 $5/2$	-0.020 $7/2$			
$n=4$	-0.203 $1/2$	-0.0781 $3/2$	-0.0365 $5/2$	-0.0156 $7/2$				
		-0.203 $1/2$	-0.0781 $3/2$	-0.0365 $5/2$				
$n=3$	-0.250 $1/2$	-0.0833 $3/2$	-0.0278 $5/2$					
		-0.250 $1/2$	-0.0833 $3/2$					
$n=2$	-0.313 $1/2$	-0.0625 $3/2$						
		-0.313 $1/2$						
$n=1$	-0.250 $1/2$							
	$l=0$	$l=1$	$l=2$	$l=3$	$l=4$			

After all this,

$l=0$: $O(p^4)$ + Darwin

$l>0$: $O(p^4)$ + Spin-Orbit

the total shift depends only
on j !!! (not which l is
the "parent")

True only to $O(\alpha^4)$

Fascinating effect at $O(\alpha^5)$...

"LAMB SHIFT" splits
the states with $l=j$ but
different "parents"

⇒ NOBEL 1955

⇒ Willis Lamb... went to
LA High School.