Ex6162: The fine structure of the Hydrogen spectrum

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The problem:

Consider the Hydrogen atom with $V_0 = -\frac{\alpha c}{r}$.
By expanding the exact solution of the Dirac equation with respect to α one obtains
$\frac{E_{n,l,j,m}}{Mc^2} = 1 - \frac{\alpha^2}{2n^2} + \frac{1}{2}(\frac{\alpha^2}{2n^2})^2[3 - \frac{4n}{j+1/2}] + ...$
Recover this expression by calculating the following corrections to the non-relativist result: The kinetic correction $W_k = -\frac{1}{8M^3c^2}p^4$, the Darwin correction $W_D = \frac{1}{8M^2c^2}\nabla^2 V_0$, and the spin-orbit correction W_s . Find also the α^5 corrections due to Lamb shift. These arise because of two reasons: an extra term $W_L = -\frac{\alpha}{15\pi M^2c^2}\nabla^2 V_0$, and an anomalous spin-orbit coupling $g \approx 2 + (\frac{\alpha}{\pi})$. All the results should be expressed in terms of and the quantum numbers (n, l, m).

The solution:

(1) the non petrubed
the rest energy is Mc^2
and the energy of the hydrogen atom is:

$$E'_n = -\frac{e^2}{2a_0n^2} = -\frac{e^2\alpha Mc}{2a_0n^2} = |e^2 = \alpha c| = -\frac{\alpha^2 Mc^2}{2n^2}$$

ther for the total unpetrubed energy is:

$$E_n = Mc^2 - \frac{Mc^2\alpha^2}{2n^2}$$

let us remmeber: $\alpha = \frac{e^2}{c\hbar}$ and $a_0 = \frac{\hbar}{Mc\alpha}$

(2) The kinetic correction:
Here we add the kinetic correction $W_k = -\frac{1}{8M^3c^2}p^4$ to the Hemiltonian

$$\mathcal{H} = \frac{p^2}{2M} + V(r) + W_k = \frac{p^2}{2M} + V(r) - \frac{1}{8M^3c^2}p^4$$

$$E^{[1]}_{n,l,j,m} = \langle nljm|W_k|n'l'j'm'\rangle = -\frac{1}{8M^3c^2}\langle nljm|P^4|n'l'j'm'\rangle =$$

$$|p^2 = (E_n - V(r))2M|$$

$$= -\frac{4M^2}{8M^3c^2}\langle nljm|((E_n - V(r)))^2|n'l'j'm'\rangle = -\frac{1}{2Mc^2}\langle nljm|E_n^2 - 2E_nV(r) + V(r)^2|n'l'j'm'\rangle =$$

$$= -\frac{1}{2Mc^2}(E_n^2\langle nljm|n'l'j'm'\rangle - 2E_n\langle nljm|V(r)|n'l'j'm'\rangle + \langle nljm|V(r)^2|n'l'j'm'\rangle) =$$

$$= \frac{1}{2Mc^2}(E_n^2 + 2E_n\left\langle\frac{\alpha c}{r}\right\rangle + \left\langle(\frac{\alpha c}{r})^2\right\rangle) =$$

according to littreture:

$$|\left\langle\frac{1}{r}\right\rangle = \frac{\alpha Mc}{\hbar n^2}, |\left\langle\frac{1}{r^2}\right\rangle = \frac{\alpha^2M^2c^2}{(l+\frac{1}{2})n^3\hbar^2}|$$

$$= -\frac{1}{2Mc^2}\left(E_n^2 + 2E_n\alpha c\frac{2Mc}{\hbar n^2} + \alpha^2c^2\frac{\alpha^2M^2c^2}{(l+\frac{1}{2})n^3\hbar^2}\right) = -\frac{1}{2Mc^2}\left(E_n^2 + 2E_n\alpha^2\frac{Mc^2}{\hbar n^2} + \alpha^4\frac{M^2c^4}{(l+\frac{1}{2})n^3\hbar^2}\right)$$

from now on $\hbar = 1$

$$E^{[1]} = -\frac{1}{2Mc^2}\left(E_n^2 + 2E_n\alpha^2\frac{Mc^2}{n^2} + \alpha^4\frac{M^2c^4}{(l+\frac{1}{2})n^3}\right) = -\frac{E_n^2}{2Mc^2}\left(1 - 2\alpha^2\frac{Mc^2}{E_n n^2} + \frac{n}{(l+\frac{1}{2})}\frac{M^2c^4\alpha^4}{n^4}\right) =$$

$$= -\frac{E_n^2}{2Mc^2}\left(1 + 2\frac{Mc^2\alpha^2}{n^2(-\frac{\alpha^2Mc^2}{2n^2})} + \frac{n}{(l+\frac{1}{2})}\frac{M^4c^4\alpha^4}{n^4\frac{\alpha^2Mc^2}{2n^2}}\right) = -\frac{E_n^2}{2Mc^2}\left(1 - 4 + \frac{n}{(l+\frac{1}{2})}\frac{\alpha^4M^2c^4}{\frac{\alpha^4M^2c^4n^4}{4n^4}}\right)$$

$$\Delta E_k = -\frac{E_n^2}{2Mc^2}\left(\frac{4n}{(l+\frac{1}{2})} - 3\right) = -\frac{\left(\frac{Mc^2\alpha^2}{2n^2}\right)^2}{2Mc^2}\left(\frac{4n}{(l+\frac{1}{2})} - 3\right) = -\frac{M^2c^4\alpha^4}{8n^4}\left(\frac{4n}{(l+\frac{1}{2})} - 3\right)$$

(3) The Darwin Term
given the darwin term $W_D = \frac{1}{8M^2c^2}\nabla^2 V_0$, Lets find the first order correction to the energies.

$$E^{[1]} = W_D = \frac{1}{8M^2c^2}\nabla^2 V_0$$

$$V_0 = -\frac{\alpha c}{r}, \quad -\nabla^2\frac{1}{r} = 4\pi\delta(r) \quad \nabla^2 V_0 = \alpha c 4\pi\delta(r)$$

$$\frac{1}{8M^2c^2}\nabla^2 V_0 = \frac{\pi\alpha}{2M^2c}\delta(r)$$

$$E^{[1]}_{n,l,j,m} = \langle nljm|W_D|n'l'j'm\rangle = \left\langle nljm|\frac{\pi\alpha}{2M^2c}\delta(r)|n'l'j'm\right\rangle = \frac{\pi\alpha}{2M^2c}\langle nljm|\delta(r)|n'l'j'm\rangle = \frac{\pi\alpha}{2M^2c}|\psi^0(0)|^2,$$

We recall that in the n,l,m basis:

$$\psi^0(0) = 0 \quad \text{for any} \quad l > 0$$

$$|\psi^0(0)|^2 = \frac{1}{\pi}\left(\frac{\alpha Mc}{n}\right)^3 \quad \text{for} \quad l = 0$$

Thus we get the correction to the energy from the Darwin term:

$$E^{[1]}_{n,l,j,m} = \frac{\pi\alpha}{2M^2c}\frac{1}{\pi}\left(\frac{\alpha Mc}{n}\right)^3 = \frac{\alpha^4Mc^2}{2\hbar^3n^3}$$

and for $\hbar = 1$:

$$\Delta E_D = \frac{\alpha^4Mc^2}{2n^3}$$

(4)The Spin Orbie correction

$$\mathcal{H} = \frac{p^2}{2M} + V(r) + W_{so} = \mathcal{H}_0 + W_{so}$$

$$W_{so} = \frac{1}{2M^2c^2r}\cdot\frac{\partial V}{\partial r}(\vec{S}\cdot\vec{L}) = -\frac{(1-g)e^2}{2M^2c^2r^3}\cdot\frac{1}{2}(J^2 - L^2 - S^2)$$

$$\langle nljms|W_{so}|n'l'j'm's'\rangle = -\frac{(1-g)e^2}{2M^2c^2}\left\langle nljms|\frac{1}{2}\frac{1}{r^3}(J^2 - L^2 - S^2)|n'l'j'm's'\right\rangle$$

$$(J^2 - L^2 - S^2)|nljms\rangle = \hbar^2[j(j+1) - l(l+1) - s(s+1)]|nljms\rangle$$

$$\left\langle nljms|W_{so}|n'l'j'm's'\right\rangle = -(1-g)(\frac{e\hbar}{2Mc})^2[j(j+1) - l(l+1) - s(s+1)]\left\langle nljms|\frac{1}{r^3}|n'l'j'm's'\right\rangle$$

$$\left\langle \frac{1}{r^3}\right\rangle = \frac{1}{a_0^3 n^3 l(l+1)(l+\frac{1}{2})} = \frac{(Mc\alpha)^3}{\hbar^3 n^3 l(l+1)(l+\frac{1}{2})}$$

for s=$\frac{1}{2}$

$$\Delta E_{so} = -(1-g)\frac{\alpha^4 Mc^2}{4n^3}\frac{j(j+1) - l(l+1) - \frac{3}{4}}{l(l+1)(l+\frac{1}{2})}$$

for s=$-\frac{1}{2}$

$$\Delta E_{so} = -(1-g)\frac{\alpha^4 Mc^2}{4n^3}\frac{j(j+1) - l(l+1) + \frac{1}{4}}{l(l+1)(l+\frac{1}{2})}$$

(5) Lamb shift:

$$\mathcal{H} = \frac{p^2}{2M} + V(r) - \frac{\alpha}{15\pi M^2c^2}\nabla^2 V_0$$

$$\left\langle nljm| - \frac{\alpha}{15\pi M^2c^2}\nabla^2 V_0|n'l'j'm'\right\rangle = -\frac{\alpha}{15\pi M^2c^2}\left\langle nlm|\nabla^2 V_0|n'l'm'\right\rangle$$

$$\nabla^2 V_0 = -\nabla^2\frac{\alpha c}{r} = \alpha c 4\pi\delta(r)$$

$$-\frac{\alpha}{15\pi M^2c^2}\left\langle nljm|\alpha c4\pi\delta(r)|n'l'j'm'\right\rangle = -\frac{\alpha^2 4\pi}{15\pi M^2c}\left\langle nljm|\delta(r)|n'l'j'm'\right\rangle = -\frac{\alpha^2 4\pi}{15\pi M^2c}|\psi_{(n,0,0)}|^2$$

according to litruture we know that for $l = 0, m = 0$

$$|\psi_{(n,0,0)}|^2 = |Y^{00}|^2|R^{n0}|^2 = \frac{1}{4\pi}|R^{n0}|^2 = \frac{1}{\pi a_0^3 n^3} = \frac{\alpha^3 M^3 c^3}{\pi\hbar^3 n^3}$$

$$\Delta E_L = -\frac{4\alpha^2}{15M^2c}\cdot\frac{\alpha^3M^3c^3}{\pi\hbar^3n^3} = -\frac{4\alpha^5 Mc^2}{15\pi\hbar^3n^3}$$

So for $\hbar = 1$ we get the term:

$$\Delta E_L = -\frac{4\alpha^5 Mc^2}{15\pi n^3}$$

(6)combination of all the terms
for $s = \frac{1}{2}$ we get $j = l + \frac{1}{2}$

$$E_n = Mc^2 - \frac{Mc^2\alpha^2}{2n^2} - \frac{Mc^2\alpha^4}{8n^4}\left(\frac{4n}{(l+\frac{1}{2})} - 3\right) + \frac{\alpha^4 Mc^2}{2n^3} - (1-g)\frac{\alpha^4Mc^2}{4n^3}\frac{j(j+1) - l(l+1) - \frac{3}{4}}{l(l+1)(l+\frac{1}{2})} - \frac{4\alpha^5 Mc^2}{\pi n^3}$$

$$= Mc^2\left(1 - \frac{\alpha^2}{2n^2} + \frac{\alpha^4}{8n^4}\left(4n + 3 - \frac{4n}{(l+\frac{1}{2})} - 2(1-g)n\cdot\frac{j(j+1) - l(l+1) - \frac{3}{4}}{l(l+1)(l+\frac{1}{2})}\right) - \frac{4\alpha^5}{\pi n^3}\right)$$

$$= 4n + 3 - \frac{4n}{j} - 2(1-g)n \cdot \frac{j(j+1) - (j-\frac{1}{2})(j+\frac{1}{2}) - \frac{3}{4}}{j(j+\frac{1}{2})(j-\frac{1}{2})}$$

$$2(1-g)n \cdot \frac{j(j+1) - (j-\frac{1}{2})(j+\frac{1}{2}) - \frac{3}{4}}{j(j+\frac{1}{2})(j-\frac{1}{2})} = 2(g-1)n \cdot \frac{j^2 + j - j^2 + \frac{1}{4} - \frac{3}{4}}{j(j+\frac{1}{2})(j-\frac{1}{2})} = 2(1-g)n \cdot \frac{j - \frac{1}{2}}{j(j+\frac{1}{2})(j-\frac{1}{2})} =$$

$$= 2(1-g)n \cdot \frac{1}{j(j+\frac{1}{2})} = 4(1-g)n \cdot \left(\frac{1}{j} - \frac{1}{(j+\frac{1}{2})}\right)$$

$g \approx 2$

$$4n \cdot \left(\frac{1}{j} - \frac{1}{(j+\frac{1}{2})}\right)$$

$$= 4n + 3 - \frac{4n}{j} + 4n \cdot \left(\frac{1}{j} - \frac{1}{(j+\frac{1}{2})}\right) = 4n + 3 - 4n\frac{1}{(j+\frac{1}{2})}$$

$$E_n = Mc^2\left(1 - \frac{\alpha^2}{2n^2} + \frac{\alpha^4}{8n^4}\left(3 + 4n\left(1 - \frac{1}{(j+\frac{1}{2})}\right)\right) - \frac{4\alpha^5}{\pi n^3}\right)$$

for $s = -\frac{1}{2}$ we get $j = l - \frac{1}{2}$

$$E_n = Mc^2 - \frac{Mc^2\alpha^2}{2n^2} - \frac{Mc^2\alpha^4}{8n^4}\left(\frac{4n}{(l+\frac{1}{2})} - 3\right) + \frac{\alpha^4 Mc^2}{2n^3} - (1-g)\frac{\alpha^4 Mc^2}{4n^3}\frac{j(j+1) - l(l+1) + \frac{1}{4}}{l(l+1)(l+\frac{1}{2})} - \frac{4\alpha^5 Mc^2}{\pi n^3}$$

$$= Mc^2\left(1 - \frac{\alpha^2}{2n^2} + \frac{\alpha^4}{8n^4}\left(4n + 3 - \frac{4n}{(l+\frac{1}{2})} - 2(1-g)n \cdot \frac{j(j+1) - l(l+1) + \frac{1}{4}}{l(l+1)(l+\frac{1}{2})}\right) - \frac{4\alpha^5}{\pi n^3}\right)$$

$$4n + 3 - \frac{4n}{(j+1)} - 2(1-g)n \cdot \frac{j(j+1) - (j+\frac{1}{2})(j+\frac{3}{2}) + \frac{1}{4}}{(j+1)(j+\frac{3}{2})(j+\frac{1}{2})}$$

$$\frac{j^2 + j - j^2 - 2j - \frac{3}{4} + \frac{1}{4}}{(j+1)(j+\frac{3}{2})(j+\frac{1}{2})} = \frac{-j - \frac{1}{2}}{(j+1)(j+\frac{3}{2})(j+\frac{1}{2})} = -\frac{1}{(j+1)(j+\frac{3}{2})} = -\frac{2}{(j+1)} + \frac{2}{(j+\frac{3}{2})}$$

$g \approx 2$

$$4n + 3 - \frac{4n}{(j+1)} - 4n \cdot \left(-\frac{1}{(j+1)} + \frac{1}{(j+\frac{3}{2})}\right) = 4n + 3 - 4n\frac{1}{(j+\frac{3}{2})} = 3 + 4n\left(1 - \frac{1}{(j+\frac{3}{2})}\right)$$

$$E_n = Mc^2\left(1 - \frac{\alpha^2}{2n^2} + \frac{\alpha^4}{8n^4}\left(3 + 4n\left(1 - \frac{1}{(j+\frac{3}{2})}\right)\right) - \frac{4\alpha^5}{\pi n^3}\right)$$