FINE STRUCTURE OF HYDROGEN: DIRAC FORMULA

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 6.19.

The fine structure of hydrogen as worked out from applying relativistic and spin-orbit coupling corrections using perturbation theory gives a formula for the energy levels as follows:

$$E_{nj} = E_{n0}\left[1-\frac{\alpha^2}{4n^2}\left(3-\frac{4n}{j+\frac{1}{2}}\right)\right] \tag{1}$$

$$= -\frac{13.6\text{ eV}}{n^2}\left[1-\frac{\alpha^2}{4n^2}\left(3-\frac{4n}{j+\frac{1}{2}}\right)\right] \tag{2}$$

If the hydrogen atom is analyzed using the relativistic Dirac equation (which we'll hopefully get to one day :)), we can get an exact formula for the energy levels:

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

Here n is the principal quantum number, j is the total angular momentum quantum number and α is the fine structure constant. We can expand this in a Taylor series in α. The derivatives are tedious and can be done using Maple, with the result

$$E_{nj} = -\frac{1}{2}\frac{mc^2}{n^2}\alpha^2-\frac{1}{8}\frac{mc^2\,(8n-6j-3)}{(1+2j)\,n^4}\alpha^4+\mathscr{O}\left(\alpha^6\right) \tag{4}$$

We can write the unperturbed energy E_{n0} in terms of α:

$$E_n = -\frac{m}{2n^2}\left(\frac{e^2}{4\pi\varepsilon_0\hbar}\right)^2 = -\frac{1}{2n^2}\alpha^2 mc^2 \tag{5}$$

Using this, we can write out the expansion as

$$E_{nj} = E_{n0} + \frac{1}{4}E_{n0}\frac{(8n-6j-3)}{(1+2j)\,n^2}\alpha^2 + \ldots \tag{6}$$

$$= \frac{E_{10}}{n^2}\left[1 + \frac{\alpha^2}{4n^2}\left(\frac{4n}{j+\frac{1}{2}} - 3\right)\right] + \ldots \tag{7}$$

$$= -\frac{13.6\text{ eV}}{n^2}\left[1 - \frac{\alpha^2}{4n^2}\left(3 - \frac{4n}{j+\frac{1}{2}}\right)\right] + \ldots \tag{8}$$

Thus the first two non-zero terms in the Taylor expansion of the Dirac formula give us the formula using perturbation theory in the non-relativistic analysis.