

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:

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

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

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:

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

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

$$E_{nj} = -\frac{1}{2} \frac{mc^2}{n^2} \alpha^2 - \frac{1}{8} \frac{mc^2 (8n - 6j - 3)}{(1 + 2j)n^4} \alpha^4 + \mathcal{O}(\alpha^6) \quad (4)$$

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

$$E_n = -\frac{m}{2n^2} \left(\frac{e^2}{4\pi\epsilon_0\hbar} \right)^2 = -\frac{1}{2n^2} \alpha^2 mc^2 \quad (5)$$

Using this, we can write out the expansion as

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

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

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

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.