LETTERS TO THE EDITORS

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Abstract. A mistake by A Sommerfeld is shown to explain the surprising agreement between his and Dirac's fine-structure formulae.

The fine structure of hydrogen atom spectral lines was discovered by A Michelson in 1887, when, his ether-wind experiments having failed, he turned to spectroscopy and found that the leading (H_α) line of the Balmer series comprises a doublet [1]. With the electron yet to be discovered, neither the nature nor, all the more, the subtle aspects of radiation had any explanation at that long ago time.

Although Bohr's 1913 atomic model did offer such an explanation ("radiation [is] emitted during the passing between different stationary states", to quote from Ref. [2]), the observed doublet structure remained unexplained because of degeneration which made Bohr levels appear as singlets.

Three more years later Sommerfeld [3] showed that in relativistic theory, energy levels split into several sublevels, with the result that radiative transitions give rise to a whole series of spectral lines (known as fine structure).

A summary of his argument is as follows: we start with the quantization rules for the so-called phase integrals [1]

$$\oint p_\varphi \, \mathrm{d}\varphi = n_\varphi h \, , \qquad \oint p_r \, \mathrm{d}r = n_r h \tag{1}$$

$(r, \varphi$ are the polar coordinates in the electron orbit plane, p_r, p_φ are their associated generalized momenta, i.e., the radial component of the momentum and the orbital moment) and then apply the relativistic energy – momentum relation

$$c^2\left(p_r^2 + \frac{L^2}{r^2}\right) + m^2 c^4 = \left(E + \frac{e^2}{r}\right)^2 , \tag{2}$$

to find the radial momentum

$$p_r = \sqrt{\frac{E^2 - m^2 c^4}{c^2} + \frac{2Ee^2}{rc^2} + \frac{e^4/c^2 - L^2}{r^2}} , \tag{3}$$

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[1] The phase integral is equal to the area enclosed by the contour of integration, so that Eqns (1) are in fact the conditions for the partition of phase space into cells of volume h^D, where D is the number of degrees of freedom. These conditions were first used by Wilson [4]; later on, Ehrenfest used the adiabatic invariance hypothesis in justifying them [5].

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and use the method of residues to evaluate the radial integral

$$I = \oint \sqrt{A + \frac{B}{r} + \frac{D}{r^2}} \, \mathrm{d}r \, .$$

We find $I = 2\pi \mathrm{i}\left(B/2\sqrt{A} + \sqrt{D}\right)$, which gives

$$2\pi \mathrm{i}\left(\frac{Ee^2}{c\sqrt{E^2 - m^2 c^4}} + \sqrt{\frac{e^4}{c^2} - L^2}\right) = n_r h \, . \tag{4}$$

Following Sommerfeld we assume
$$L^2 = p_\varphi^2 = n_\varphi^2 \hbar^2 \, , \tag{5}$$

to give

$$E = mc^2 \left[1 + \left(\frac{\alpha}{n_r + \gamma}\right)^2\right]^{-1/2} , \quad \alpha = \frac{e^2}{\hbar c} \, , \quad \gamma = \sqrt{n_\varphi^2 - \alpha^2} \, . \tag{6}$$

Expanding in a power series of the fine-structure constant $\alpha = 1/137$ we arrive at

$$E_{n, n_\varphi} = mc^2 - \frac{\Re\mathrm{y}}{n^2} + \frac{\alpha^2 \Re\mathrm{y}}{n^4}\left(\frac{3}{4} - \frac{n}{n_\varphi}\right) + \dots , \quad n = n_r + n_\varphi \, . \tag{7}$$

Here, the first term is the rest energy, while the second, the Bohr binding energy (n is the principal quantum number, $\Re\mathrm{y} = mc^2 \alpha^2/2$ is the Rydberg constant), and the third, a relativistic correction. It is the dependence of this correction on n_φ, which removes the degeneracy of Bohr's model.

The second level of the hydrogen atom splits into two sublevels, corresponding to $n_\varphi = 1$ and 2 (2S and 2P in modern notation), with $E_{22} - E_{21} = \alpha^2 \Re\mathrm{y}/16$. The level splitting is easily traced to the $(e^2/r)^2$ correction to the potential energy [see Eqn (2)]. The same term causes a rotation of the perihelion of the orbit.

For almost 12 years, the Sommerfeld formula was considered the only correct one. Even after the creation of quantum mechanics, the calculations based on relativistic (spinless) Klein – Gordon wave equation gave the formula

$$\Delta E_{nl}^{(\mathrm{KG})} = \frac{mc^2 \alpha^4}{2n^4}\left(\frac{3}{4} - \frac{n}{l + 1/2}\right) , \tag{8}$$

yielding a splitting $\alpha^2 \Re\mathrm{y}/6$, which is 8/3 times the correct value. [2]

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[2] Folklore has it [6] that this formula was first derived by E Schrödinger... Having written a relativistic equation with a Coulomb field in the fall of 1925, he laid aside the equation when he saw the resulting fine structure to be wrong. Some time later, however, he realized that a nonrelativistic calculation is viable as well and published it in January 1926, making no mention of relativism, though...

The discovery of the spin had a two-fold effect on Sommerfeld's theory. First, the appearance of a third quantum number j changed the classification of the levels (in particular, the second level is represented by three sublevels $2S_{1/2}$, $2P_{1/2}$, $2P_{3/2}$) and, second, the spin-orbit interaction had to be taken into account. At that point, a small miracle occurred: Heisenberg and Jordan [7] and then Darwin [8] showed that this interaction, together with the spinless term $\Delta E_{nl}^{(KG)}$, leads to the formula

$$\Delta E_{nj} = \frac{mc^2\alpha^4}{2n^4}\left(\frac{3}{4} - \frac{n}{j + 1/2}\right), \qquad (9)$$

which gives the same answer as Sommerfeld's 'old' formula (7).

In the truth, when adding the orbital and spin momenta, the values of j run from $l_{\min} + 1/2 = 1/2$ to $l_{\max} + 1/2 = n - 1/2$, so that $1 \leqslant j + 1/2 \leqslant n$. Because this spectrum coincides with that of the values of n_φ — both varying from 1 to n — the numerical results of both theories are the same. [3]

Furthermore, early in 1928 the same formula (9) was obtained by P Dirac working (perturbatively[4]) within a consistent quantum-relativistic theory with spin. In the same year, Darwin [10] and Gordon [11] exactly solved the Dirac equation with the Coulomb potential to obtain an energy level formula of the form

$$E = mc^2\left[1 + \left(\frac{\alpha}{n_r + \gamma_D}\right)^2\right]^{-1/2}, \qquad \gamma_D = \sqrt{(j + 1/2)^2 - \alpha^2}. \qquad (10)$$

As can be seen, this formula has the same form as Sommerfeld formula (6) — except for the fundamental difference that n_φ is replaced by $j + 1/2$.

So, a paradoxical situation arose in which an eclectic theory somehow turned out to be equivalent to the consistent Dirac theory, which it should not because, if for no other reason, Sommerfeld had not taken into account the spin-orbit interaction — that is, a relativistic effect of the same order as what his theory included. In the work cited above, Sommerfeld also attempted to explain the anomalous Zeeman effect, but met with no success because this cannot be done without spin taken into account.

There are differing opinions in the scientific literature as to what may be the reason for the equivalence. For some, the mutual compensation for the spin contribution and wave effects is the answer [12]. This is wrong, however, because wave properties are included indirectly in Sommerfeld's work: he actually worked in the quasi-classical approximation when writing the quantization rules (1). Therefore, there is simply nothing for spin to compensate with. Others consider this situation to be 'an absolutely chance coincidence' — such are, in particular, the words with which Weinberg [13] concludes his review of the situation; while he

shows that the sum $\Delta E_{nl}^{(KG)} + \Delta E_{\text{sp-orb}}$ is equal to ΔE_{Somm}, no analysis is given of this fact. In older books [14], Sommerfeld's theory is usually criticized for wrongly classifying energy levels and for selection rules, but, while using Eqn (7), the authors of these books remain silent about its 'strangeness'. Heisenberg calls the coincidence a 'miracle' and writes "It would be intriguing to explore whether this is about a miracle or it is the group-theoretical approach which leads to this formula" [15]. A radical attempt at resolving the situation was that by Biedenharn [16] who noted that when one transforms to a rotating coordinate system, an analogy can be drawn between the classical solution of Sommerfeld and Dirac's quantum solution. Unfortunately, Biedenharn's failure to transform the Hamiltonian function took away much of the value of his work.

The answer, however, is fairly simple if one comes to think of it: the coincidence is due to Sommerfeld [5] mistakenly replacing the square of the orbital moment L^2 by $L_z^2 = n_\varphi^2\hbar^2$ in Eqn (4). In the quasi-classical approximation, $L^2 = (l + 1/2)^2\hbar^2$ is a correct result, so that if Sommerfeld 'did good science', then his formula would contain $l + 1/2$ instead of n_φ — leading to a splitting of $\alpha^2 \Re y/6$ nearly three times larger. In this way, he would arrive at the Schrödinger – Klein – Gordon result — as appropriate for the spinless case.

And it was a deeply hidden error which led to a correct answer!

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[3] Note a disagreement in definitions, though. While with Sommerfeld, fine structure is the splitting of the levels 2S and 2P that differ in parity, with Dirac $2P_{1/2}$ and $2P_{3/2}$ are of the same parity. True, the levels $2S_{1/2}$ and $2P_{1/2}$ are degenerate only to within radiation corrections: it is in the study of fine structure that the Lamb shift of the hydrogen $2S_{1/2}$ level was discovered [9].

[4] Dirac was afraid, he avowed, that higher order approximations would worsen agreement with experiment, as was the case with Schrödinger (see footnote 2).

[5] In quantum theory, unlike in classical theory, there is no such thing as an orbit's plane, so that the square of moment does not reduce to the square of L_z: although the component L_z is still conserved, there also exist L_x, L_y, whose squares are nonzero.