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The relativistic nature of hydrogen

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Abstract: In this article I will show how clear the connection is between hydrogen's fine-structure is to the special theory of relativity. We'll conclude that a quantum version of the Lorentz-factor is needed and that it will reduce to the classical description of the energy levels. In the calculations a new energy has appeared and how this energy is to be interpreted is open to debate.

1.1 Introduction

The finestructure of hydrogen is due to the first order of relativistic correction to the electrons kinetic energy and the spin-orbital effect. Under high resolution experiments the different energy levels are actually more complicated than first observed by classical measurement. But the problem of the nonexistents of relativistic correction was already well known in the early days of quantum mechanics, because the Schrodinger equation is purely classical. Though is must be said that the classical description of the hydrogen atom is a good approximation for most.

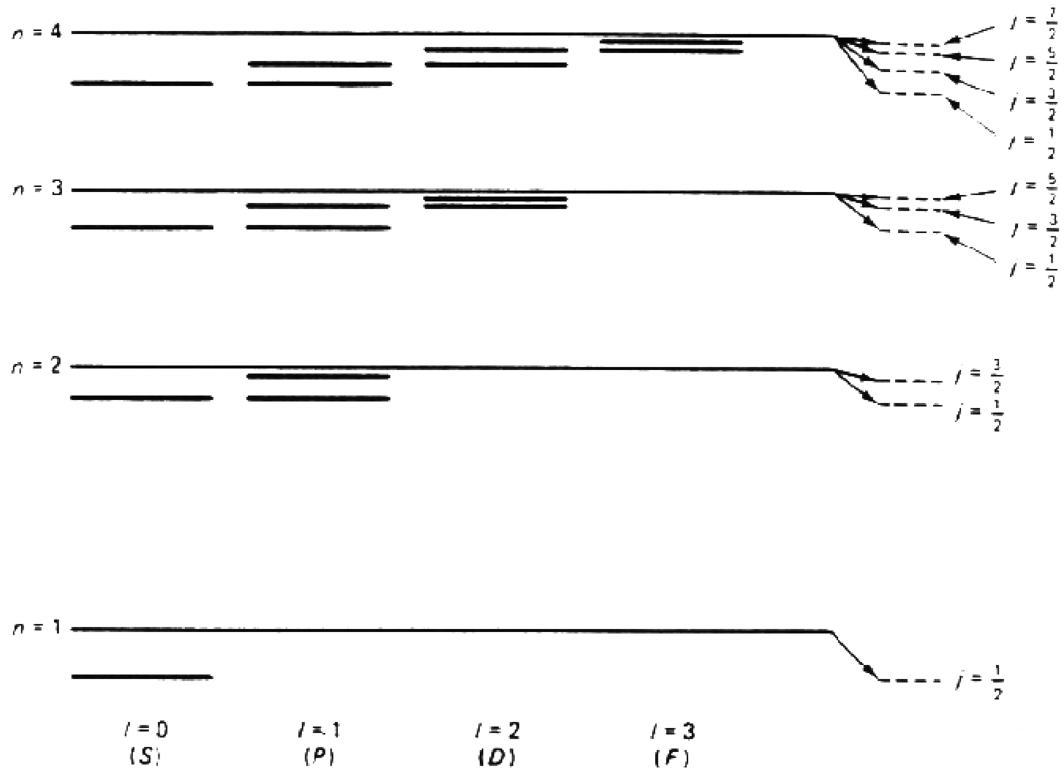

Figure 1

The figure[1] illustrates the energy levels of the hydrogen atom at different states depending on the principal quantum number.

The (first order)-relativistic correction due to the electrons kinetic energy is given by[2]

$$\Delta E_{nl} = E_n \frac{\alpha^2}{n^2}\left(\frac{n}{l+½} - \frac{3}{4}\right) \tag{1}$$

Where $n \geq 1$ is the principal quantum number and $0 \leq l \leq n-1$ is the electrons orbital (azimuthal) quantum number and:

$$E_n = -\frac{E_R}{n^2} \tag{2}$$

The correction due to the spin-orbital effect is given by[2]

$$\Delta E_{lj} = E_n \frac{\alpha^2}{n^2}\left(\frac{n\left[\frac{3}{4} + l(l+1) - j(j+1)\right]}{2l(l+½)(l+1)}\right) \tag{3}$$

Now adding equations (1) and (3) we will get the net correction to the energy levels of hydrogen atom

$$\Delta E_{nj} + = \Delta E_{nl} + \Delta E_{lj} \Leftrightarrow \Delta E_{nj} = E_n \frac{\alpha^2}{n^2}\left(\frac{n}{j+½} - \frac{3}{4}\right) \tag{4}$$

Where we used the fact that $j = l \pm ½$. This is actually quite easy to understand. The electron spin can either be +½ or -½ and since it's "orbiting" the nucleus with an angular momentum *L*. The total angular momentum must then be the sum of these two. All of this means that energy levels of hydrogen atom are given by the equation

$$E_{nj} = E_n + \Delta E_{nj} \Leftrightarrow E_{nj} = E_n\left(1 + \frac{\alpha^2}{n^2}\left[\frac{n}{j+½} - \frac{3}{4}\right]\right) \tag{5}$$

From Paul Dirac's theory one can show that hydrogens total energy are equal to

$$E_{nj} = \frac{m_e c^2}{\sqrt{1 + \frac{\alpha^2}{\left[n - (j + ½) + \sqrt{(j + ½)^2 - \alpha^2}\right]^2}}} \tag{6}$$

Now by using the Binomial theorem one gets

$$E_{nj} = m_e c^2 + E_n + E_n \frac{\alpha^2}{n^2} \left(\frac{n}{j + ½} - \frac{3}{4} \right) + \ldots \tag{7}$$

And equation (7) shows that equation (5) is only the third order approximation to the energy or the second order to the kinetic energy

$$W_{nj} = E_{nj} - m_e c^2 \Leftrightarrow W_{nj} = E_n + E_n \frac{\alpha^2}{n^2} \left(\frac{n}{j + ½} - \frac{3}{4} \right) + \ldots \tag{8}$$

Now equation (5) is interesting because it has some similarity to the total relativistic energy of a particle

$$E = E_0 \gamma(v) \tag{9}$$

Where $E_0 = m_0 c^2$ is the resting energy of the particle. Now the interesting question is, if the factor in equation (5) is the quantum version of the Lorentz factor. One thing we do now about equation (5) is that it must be Lorentz invariant. That is because, the correction made to the energy levels are well within the special theory of relativity. The following investigations will maybe enlighten these aspects.

1.2 A simple assumption

For the sake of simplicity I will consider an incorrect scenario. I will make the classical assumption, that the electron orbits the proton in a uniform circular motion with and relativistic momentum p at a distance r from the proton. This means that its angular momentum is given by

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \tag{10}$$

Since the electron is in a circular orbit the magnitude of the angular momentum is then given by

$$L = r m_0 v \gamma(v) \tag{11}$$

Where $p = m_0 v \gamma(v)$ is the relativistic momentum. Now by applying the simple quantum condition

$$r_n m_0 v_n \gamma_n(v_n) = n\hbar Y_{nj} \tag{12}$$

We are then able to calculate some useful relations. The function Y is some unknown function of the principal quantum number and the total orbital quantum number. Equation (12) can be written as

$$r_n m_0 \frac{v_n}{\sqrt{1 - \frac{v_n^2}{c^2}}} = n\hbar Y_{nj} \tag{13}$$

What we are interested in, is isolating the velocity and then "remake" the Lorentz factor. We can do this in two ways that will yield a very important equation. By squaring equation (13) we'll get

$$(r_n m_0)^2 \frac{v_n^2}{1 - \frac{v_n^2}{c^2}} = n^2 \hbar^2 Y_{nj}^2 \tag{14}$$

If we make some rearrangement of terms we'll get

$$\frac{v_n^2}{1 - \frac{v_n^2}{c^2}} = c^2 \frac{\lambda_n^2}{r_n^2} Y_{nj}^2 \tag{15}$$

Now the electrons Compton wavelength are introduced in a new way by the equation

$$\lambda_n = \lambda_C n \tag{16}$$

Equation (15) can now be rewritten as

$$\frac{v_n^2}{c^2} = \frac{\lambda_n^2}{r_n^2} Y_{nj}^2 - \frac{v_n^2}{c^2}\frac{\lambda_n^2}{r_n^2} Y_{nj}^2 \Leftrightarrow \frac{v_n^2}{c^2}\left(1 + \frac{\lambda_n^2}{r_n^2} Y_{nj}^2\right) = \frac{\lambda_n^2}{r_n^2} Y_{nj}^2 \tag{17}$$

This means

$$1 - \frac{v_n^2}{c^2} = 1 - \frac{\lambda_n^2}{r_n^2} Y_{nj}^2 \left(1 + \frac{\lambda_n^2}{r_n^2} Y_{nj}^2\right)^{-1} \tag{18}$$

The right side of equation (18) can be rewritten the following way

$$1 - \frac{\lambda_n^2}{r_n^2} Y_{nj}^2 \left(1 + \frac{\lambda_n^2}{r_n^2} Y_{nj}^2\right)^{-1} = \frac{1 + \frac{\lambda_n^2}{r_n^2} Y_{nj}^2 - \frac{\lambda_n^2}{r_n^2} Y_{nj}^2}{1 + \frac{\lambda_n^2}{r_n^2} Y_{nj}^2} \tag{19}$$

Equation (18) is then equal to

$$1 - \frac{v_n^2}{c^2} = \frac{1}{1 + \frac{\lambda_n^2}{r_n^2} Y_{nj}^2} \tag{20}$$

Or just

$$\frac{1}{\gamma_{nj}^2} = \frac{1}{1 + \frac{\lambda_n^2}{r_n^2} Y_{nj}^2} \Leftrightarrow \gamma_n^2 = 1 + \frac{\lambda_n^2}{r_n^2} Y_{nj}^2 \tag{21}$$

Now according to quantum mechanics we are able to calculate the expectation value for the electrons position in some distance r from the proton. This can be done by considering $|\psi|^2$ as the probability density pr. unit length, and therefore the expectations values for $\langle r^k \rangle$ can be found by solving the integral[3]

$$\langle r^k \rangle = \int_0^\infty r^k \left| R(r) \right|^2 dr \tag{22}$$

We know that the electron is in a central potential V that depends on the distance r by $V(r) \propto r^{-1}$ which means that equation must be written as

$$\gamma_{nj}^2 = 1 + \lambda_n^2 \langle r^{-1} \rangle^2 Y_{nj}^2 \tag{23}$$

By some tedious calculations we are able to confirm that

$$\langle r^{-1} \rangle = \frac{1}{n^2 a_0} \tag{24}$$

Where

$$a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{me^2} \tag{25}$$

Is the Bohr-radius. Now by using equation (16) and inserting (24) into equation (23) we'll get

$$\gamma_{nj}^2 = 1 + \frac{\lambda_C^2}{n^2 a_0^2} Y_{nj}^2 \tag{26}$$

Now the ratio between the electrons Compton wavelength and the Bohr distance reveals the fine structure constant

$$\frac{\lambda_C}{a_0} = \frac{\hbar}{m_e c} \frac{me^2}{4\pi\varepsilon_0 \hbar^2} \Leftrightarrow \alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c} \tag{27}$$

Which means that equation (26) can elegantly be written as

$$\gamma_{nj}^2 = 1 + \frac{\alpha^2}{n^2} Y_{nj}^2 = 1 + \alpha^2 B_{nj} \tag{28}$$

Where $B_{nj} := Y_{nj}^2 / n^2$. Now it can easily be shown that

$$\gamma_{nj}^2 = 1 + Z^2 \frac{\alpha^2}{n^2} Y_{nj}^2 = 1 + Z^2 \alpha^2 B_{nj} \tag{29}$$

Where Z is the number of nucleons, but further in this article we'll use $Z = 1$. By comparing equation (28) and (5) we see that the unknown function Y is given by

$$Y_{nj}^2 := \frac{n}{j + ½} - \frac{3}{4} \tag{30}$$

The significance of equation (28) is that it *directly* connects the relativistic effects of the electrons motion to the most characteristic scalar in Einstein's theory. This is not obvious by just looking at equation(5). Although we might have "guessed it". Like I mentioned earlier there were two ways to do these calculations and by returning to equation (13), we can rewrite this as followed

$$r_n \gamma_n (v_n) = n \frac{\hbar}{m_0 v_n} Y_{nj} \Leftrightarrow \gamma_n^2 = \frac{\lambda_{Bn}^2}{r_n^2} Y_{nj}^2 \tag{31}$$

Where

$$\lambda_{Bn} = \frac{\hbar}{p_{0n}} n \tag{32}$$

1.3 The de Broglie equation

Now measuring the de Broglie wavelength of particle is very difficult, and therefore we are looking for a connection in equation (32) to the kinetic energy of the particle. In classical mechanics we know that

$$\lambda = \frac{hc}{\sqrt{2Km_0c^2}} \tag{33}$$

But since we are taking account for relativistic effects the classical equation for the kinetic energy is therefore not valid. Another thing we have to mention is that the momentum appearing in equation (32), is the relativistic momentum which means we have to include the Lorentz factor in equation (32)

$$\lambda_{Bn} = \frac{\hbar}{p_{0n}\gamma_n}\gamma_n n \tag{34}$$

By taking account for the relativistic momentum and kinetic energy of the particle, we are then able to derive the following equation

$$p = m_0 v \frac{K + E_0}{E_0} \tag{35}$$

Where $E_0 = m_0 c^2$ and

$$\gamma = \frac{K + m_0 c^2}{m_0 c^2} \tag{36}$$

Equation (36) relates the particles kinetic energy and rest energy to the Lorentz factor which means that

$$\frac{K + E_0}{E_0} = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} \tag{37}$$

By solving equation (37) in term of v equation (35) can therefore be rewritten as

$$p = \frac{K + E_0}{c}\sqrt{1 - \left(\frac{K}{E_0} + 1\right)^{-2}} \tag{38}$$

If we perform the algebra and reduce equation (38) then we'll get

$$cp = \sqrt{K^2 + 2KE_0} \tag{39}$$

From equation (39) it is easy to identify the relativistic version of equation (33) because

$$\lambda = \frac{hc}{\sqrt{K^2 + 2KE_0}} \tag{40}$$

By assuming that the particles kinetic energy is much smaller than its resting energy (that is $K \ll E_0$), equation (40) will reduce to the classical equation. According to our assumptions, the kinetic energy of the electron must be quantized, because the radius at which it is "located" depends on the principal quantum number and therefore its "velocity" must be different as well. This means that equation (34) is equal to

$$\lambda_{Bn} = \frac{\hbar c}{\sqrt{K_n^2 + 2K_n E_0}} \left(\frac{K_n}{E_0} + 1 \right) n \tag{41}$$

By inserting equation (41) back into equation (31) we'll get

$$\gamma_{nj}^2 = \left(\frac{\hbar c}{r_n} \right)^2 \frac{n^2 Y_{nj}^2}{K_n^2 + 2K_n E_0} \left(\frac{K_n}{E_0} + 1 \right)^2 \tag{42}$$

And by using equation (24) and inserting into equation (42), it can be written as follows

$$\gamma_{nj}^2 = \left(\frac{\hbar c}{a_0} \right)^2 \frac{B_{nj}}{K_n^2 + 2K_n E_0} \left(\frac{K_n}{E_0} + 1 \right)^2 \tag{43}$$

The constant appearing in equation (43) has the unit of energy and will be denoted by the symbol

$$\kappa_0 := \frac{\hbar c}{a_0} \tag{44}$$

Equation (43) can finally be written as

$$\gamma_{nj}^2 = \frac{\kappa_0^2 B_{nj}}{K_n^2 + 2K_n E_0}\left(\frac{K_n}{E_0} + 1\right)^2 \tag{45}$$

If equation (45) and equation (28) are equal, then we must add a condition for the kinetic energy, i.e. we need to solve the following equation

$$1 + \alpha^2 B_{nj} = \frac{\kappa_0^2 B_{nj}}{K_n^2 + 2K_n E_0}\left(\frac{K_n}{E_0} + 1\right)^2 \tag{46}$$

For the sake of simplicity we denoted, for the time being, $\gamma_n^2 = C_{nj}$ so that equation (46) is equal to

$$C_{nj} = \frac{\kappa_0^2 B_{nj}}{K_n^2 + 2K_n E_0}\left(\frac{K_n}{E_0} + 1\right)^2 \tag{47}$$

By doing the algebra on equation (47) we'll get the following quadratic equation with some rather grim looking coefficients

$$\left(\tfrac{\kappa_0^2 B_{nj}}{E_0^2} - C_{nj}\right)K_n^2 + 2\left(\tfrac{\kappa_0^2 B_{nj}}{E_0} - E_0 C_{nj}\right)K_n + \kappa_0^2 B_{nj} = 0 \tag{48}$$

Solving this equation turns out to be quite easy. The discriminant is equal to

$$D = 4\left(\tfrac{\kappa_0^2 B_{nj}}{E_0} - E_0 C_{nj}\right)^2 + 4\left(C_{nj} - \tfrac{\kappa_0^2 B_{nj}}{E_0^2}\right)\kappa_0^2 B_{nj} \tag{49}$$

By reducing equation (49) we'll get simple equation

$$D = 4C_{nj}\left(E_0^2 C_{nj} - \kappa_0^2 B_{nj}\right) \tag{50}$$

This means we'll get the following solutions

$$K_{n1,n2} = \frac{\left(E_0 C_{nj} - \frac{\kappa_0^2 B_{nj}}{E_0}\right) \pm \sqrt{C_{nj}\left(E_0^2 C_{nj} - \kappa_0^2 B_{nj}\right)}}{\frac{\kappa_0^2 B_{nj}}{E_0^2} - C_{nj}} \tag{51}$$

By doing a little algebra, equation (51) can be reduced to

$$\begin{aligned} K_{n1,n2} &= \frac{\left(E_0^3 C_{nj} - \kappa_0^2 B_{nj} E_0\right) \pm E_0^2 \sqrt{C_{nj}\left(E_0^2 C_{nj} - \kappa_0^2 B_{nj}\right)}}{\left(\kappa_0^2 B_{nj} - C_{nj} E_0^2\right)} \Leftrightarrow \\ K_{n1,n2} &= -E_0 \pm E_0^2 \sqrt{\frac{C_{nj}}{E_0^2 C_{nj} - \kappa_0^2 B_{nj}}} \Leftrightarrow \\ K_{n1,n2} &= -E_0 \pm \frac{E_0}{\sqrt{1 - \frac{\kappa_0^2 B_{nj}}{E_0^2 C_{nj}}}} \end{aligned} \tag{52}$$

1.4 The classical limit

Equation (52) states that there are two solutions, but if the kinetic energy is relativistic in nature, then it's obvious that the positive solution is the correct one. This means that

$$K_n = \frac{E_0}{\sqrt{1 - \frac{\kappa_0^2 B}{E_0^2 C}}} - E_0 \tag{53}$$

Now if this solution is identical to the relativistic version of the kinetic energy have to require that

$$C_{nj} = \frac{1}{1 - \frac{\kappa_0^2 B_{nj}}{E_0^2 C_{nj}}} \tag{54}$$

Now by solving this equation we'll get

$$C_{nj} = 1 + \frac{\kappa_0^2}{E_0^2} B_{nj} \tag{55}$$

And this means that

$$1 + \alpha^2 B_{nj} = 1 + \frac{\kappa_0^2}{E_0^2} B_{nj} \tag{56}$$

The consequence of the this result requires

$$\alpha = \frac{\kappa_0}{m_0 c^2} \Leftrightarrow m_0 = m_e \tag{57}$$

So that

$$K_n = E_0 \gamma_n - E_0 \tag{58}$$

Now to investigate the classical limit we have to use the binomial theorem on equation(58). This will yield

$$K_n \simeq E_0 \left(1 + \tfrac{1}{2}\alpha^2 B_{nj} - \tfrac{1}{8}\alpha^4 B_{nj}^2 + \ldots\right) - E_0 \tag{59}$$

Since the fine-structure constant is very small for higher-orders of approximation, we can neglect these terms and get

$$K_n = \tfrac{1}{2} E_0 \alpha^2 B_{nj} \tag{60}$$

If we perform the same approximation on equation (53) we'll get

$$K_n \simeq E_0 \left(1 + \tfrac{\kappa_0^2 B_{nj}}{2E_0^2 C_{nj}} + \tfrac{\kappa_0^4 B_{nj}^2}{8E_0^2 C_{nj}^2} + \ldots\right) - E_0 \Rightarrow K_n \approx \tfrac{\kappa_0^2 B_{nj}}{2E_0 C_{nj}} \tag{61}$$

According to the calculations from equation (54) through (57) we've establish that the ratio on the energies appearing in equation(61), are identical to the fine-structure constant and this means that

$$\frac{\kappa_0^2 B_{nj}}{2E_0 C_{nj}} \approx \frac{1}{2} E_0 \alpha^2 B_{nj} \Leftrightarrow C_{nj} \approx \frac{\kappa_0^2}{E_0^2 \alpha^2} \Leftrightarrow C_{nj} \approx 1 \tag{62}$$

Since we've establish that there is a link to the Lorentz-factor in equation (5) we are able to conclude that the equation, reduces to the classical result for the energy levels of hydrogen.

1.5 Conclusion

In this article we have showed that the factor appearing in equation (58) (and equation (29)) can be considered to be a quantum version of the Lorentz factor, and that the square of this factor are related to the energy levels described in equation (5). We've also showed that it has the correct classical limit. Another interesting thing is, that ration between the electrons rest mass and the energy defined in equation (44) gives the fine-structure constant. This bring us directly to equation (57) which can be written as

$$\alpha = \frac{m_\kappa}{m_0} \tag{63}$$

Where $m_\kappa = \kappa_0 / c^2$. Now if $m_0 = m_e$ then equation (63) are equal to the fine-structure constant, but equation (63) states that this doesn't always have to be case. For years it has been debated if the fine-structure constant has been maintaining the same value since the beginning of time. But for now (2010) it's still commonly believed that it is a true constant of nature.

The mass/energy represented in the equation is somewhat a mystery. It could be just a coincidence that a energy is represented there. If we were a bit bold it could be the mass of a new particle that has the same properties as the electron, but has a mass that's around a hundred times smaller. Now some theories have postulated the existence of super symmetry, which basically means that every particle has a more massive partner, but in this case though it seems to be the other way around.

1.6 References

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