**A look at Sommerfeld's fine structure spectrum formula**

Jorma Jormakka
Vantaa, Finland
jorma.o.jormakka@gmail.com

Abstract: The article gives the derivation of Sommerfeld's fine structure spectrum formula and my comments on it. I think Sommerfeld's approach has been too easily discarded.

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## 1. From the classical Kepler problem to Sommerfeld's equation

Kepler concluded that the angular momentum $p_\phi = mr^2\dot{\phi}$ is constant in planet's orbits. This is true for situations where a mass $m$ is circulating a Coulomb-type potential

$$V = -\frac{g}{r}. \tag{1}$$

The classical Hamiltonian is

$$E = \frac{p^2}{2m} + V. \tag{2}$$

The total momentum can be expressed with the radial and angular parts:

$$p^2 = p_r^2 + \frac{1}{r^2}p_\phi^2 \tag{3}$$

where $p_\phi$ is constant because of the conservation of angular momentum, and $p_r$ can be expressed by using $p_\phi$ as

$$p_r = m\dot{r} = m\frac{dr}{dt} = m\frac{d\phi}{dt}\frac{dr}{d\phi} = \frac{1}{r^2}mr^2\dot{\phi}\frac{dr}{d\phi} = \frac{1}{r^2}p_\phi\frac{dr}{d\phi}. \tag{4}$$

Let $s = \frac{1}{r}$. As

$$\frac{d}{d\phi}\frac{1}{r} = -\frac{1}{r^2}\frac{dr}{d\phi} \quad \rightarrow \quad \left(\frac{1}{r^2}\frac{dr}{d\phi}\right)^2 = \left(\frac{ds}{d\phi}\right)^2. \tag{5}$$

Thus

$$p^2 = p_\phi^2\left(\frac{ds}{d\phi}\right)^2 + s^2p_\phi^2 \tag{6}$$

and

$$E - V = \frac{p^2}{2m} \tag{7}$$

gives

$$\left(\frac{ds}{d\phi}\right)^2 + s^2 = \frac{2m}{p_\phi^2}(E + gs) \tag{8}$$

which can be solved e.g. by derivating with respect to $\phi$

$$2\frac{ds}{d\phi}\left(\frac{d^2s}{d\phi^2}\right)+2\frac{ds}{d\phi}s=\frac{ds}{d\phi}\frac{2m}{p_\phi^2}g \tag{9}$$

$$\frac{d^2s}{d\phi^2}+s-\frac{m}{p_\phi^2}g=0. \tag{10}$$

The general solution of this kind of an equation is

$$s=A+C_1\sin(\phi)+C_2\cos(\phi) \tag{11}$$

and the solution to the Kepler problem is an ellipse. In polar coordinates the equation of an ellipse is

$$\frac{1}{s}=r=\frac{1+\epsilon\cos(\phi)}{a(1-\epsilon^2)} \tag{12}$$

where $a$ is the semimajor and $b$ the semiminor axis and $\epsilon=\sqrt{1-(b/a)^2}$ is the eccentricity. In Cartesian coordinates the ellipse (12) is

$$\left(\frac{x+\epsilon a}{a}\right)^2+\left(\frac{y}{b}\right)^2=1, \tag{13}$$

the origin is at the left focal point $(-ea,0)$.

Sommerfeld generalized the ellipse to

$$r=\frac{1+\epsilon\cos(\omega\theta)}{a(1-\epsilon^2)} \tag{14}$$

where $\theta=\omega\phi$, $p_r=m\dot{r}$, $p_\theta=mr^2\dot{\theta}$. Similarly as before

$$p_r=\frac{1}{r^2}p_\theta\frac{dr}{d\phi}. \tag{15}$$

This ellipse precesses. It does not solve the the classical Hamiltonian (2) if $\omega\neq 1$. The problem can be seen by inserting the precessing ellipse equation and calculating:

$$p_r=m\dot{r}=\dot{\theta}\frac{d}{d\theta}\frac{a(1-\epsilon^2)}{1+\epsilon\cos(\omega\theta)}=m\dot{\theta}\frac{a(1-\epsilon^2)}{(1+\epsilon\cos(\omega\theta))^2}\epsilon\omega\sin(\omega\theta) \tag{16}$$

$$=m\dot{\theta}\left(\frac{a(1-\epsilon^2)}{1+\epsilon\cos(\omega\theta)}\right)^2\frac{1}{a(1-\epsilon^2)}\epsilon\omega\sin(\omega\theta) \tag{17}$$

$$=mr^2\dot{\theta}\frac{1}{a(1-\epsilon^2)}\sin(\omega\theta)=p_\theta\frac{1}{a(1-\epsilon^2)}\epsilon\omega\sin(\omega\theta). \tag{18}$$

We get

$$p_r^2=p_\theta^2\frac{\epsilon^2\omega^2}{(a(1-\epsilon^2))^2}(1-\cos^2(\omega\theta)) \tag{19}$$

$$\frac{1}{r^2}p_\theta^2 = p_\theta^2\left(\frac{1+\epsilon\cos(\omega\theta)}{a(1-\epsilon^2)}\right)^2. \tag{20}$$

Thus

$$p^2 = p_r^2 + \frac{1}{r^2}p_\theta^2 = p_\theta^2\frac{1}{(a(1-\epsilon^2)^2}(1+\epsilon^2\omega^2) \tag{21}$$

$$+ p_\theta^2\frac{2\epsilon}{(a(1-\epsilon^2)^2}\cos(\omega\theta) \tag{22}$$

$$+ p_\theta^2\frac{\epsilon^2}{(a(1-\epsilon^2)^2}(1-\omega^2)\cos^2(\omega\theta). \tag{23}$$

The problem is that the potential

$$V = g\frac{a(1-\epsilon^2)}{1+\epsilon\cos(\omega\theta)} \tag{24}$$

does not have a $\cos^2(\omega\theta)$ term and it cannot cancel this term in the kinetic energy in order to get constant $E$ in the classical Hamiltonian.

There is a mathematical trick that can be done to allow precessing ellipses as solutions: square the potential energy in order to get the $\cos^2(\omega\theta)$ term. We can write with any number $w$

$$\frac{p^2}{2m} = \lim_{w\to\infty}(\sqrt{p^2w + m^2w^2} - mw) \tag{25}$$

because

$$mw\sqrt{1+\frac{p^2}{m^2w}} - mw = mw\left(\frac{1}{2}\frac{p^2}{m^2w} + O(w^{-2})\right). \tag{26}$$

With this trick the Hamiltonian takes the form

$$(E + m^2w^2 + V)^2 = p^2w + m^2w^2 \tag{27}$$

where $w$ is a large number so that the kinetic energy

$$K = \sqrt{p^2w + mw^2} - mw \tag{28}$$

is sufficiently close the original kinetic energy $p^2/m$. Equation (27) is satisfied for $\omega \neq 1$ as we introduced the $\cos^2$ term. This is simply a mathematical trick and it does not require that $p = \gamma mv$ where $\gamma$ is the Lorentz factor, or any relativity theory at all.

The relativistic kinetic energy formula (where $w = c^2$, $m = m_0$, $p = \gamma m_0 v$ and $E$ includes $m_0c^2$) is

$$(E + V)^2 = p^2c^2 + m_0^2c^4. \tag{29}$$

It makes this trick. Sommerfeld used the relativistic energy formula, we will discuss it in Section 3.

## 2. Derivation of Sommerfeldt's fine structure spectrum formula

The following derivation is not the way Sommerfeld derived the formula. It is based on the easier derivation in [1]. I give also the last step which [1] describes as "tedius but straightforward" as it took me quite some time to make this step.

Starting from

$$(E+V)^2 = p^2c^2 + m_e^2c^4 \tag{30}$$

and inserting

$$r = \frac{a(1-\epsilon^2)}{1+\epsilon\cos(\omega\theta)} \tag{31}$$

yields the equations

$$\left(E^2 + \frac{g}{a(1-\epsilon^2)})\right)^2 \tag{32}$$

$$+ Eg\frac{2\epsilon}{a(1-\epsilon^2)}\cos(\omega\theta) + g^2\frac{2\epsilon}{(a(1-\epsilon^2)^2}\cos(\omega\theta) \tag{33}$$

$$+ g^2\frac{\epsilon^2}{(a(1-\epsilon^2)^2}\cos^2(\omega\theta) = \tag{34}$$

$$p_\theta^2c^2\frac{1}{(a(1-\epsilon^2)^2}(1+\epsilon^2\omega^2) + m_e^2c^4 \tag{35}$$

$$+ p_\theta^2c^2\frac{2\epsilon}{(a(1-\epsilon^2)^2}\cos(\omega\theta) \tag{36}$$

$$+ p_\theta^2c^2\frac{\epsilon^2}{(a(1-\epsilon^2)^2}(1-\omega^2)\cos^2(\omega\theta). \tag{37}$$

Matching the powers of $\cos(\omega\theta)$ gives

$$\omega^2 = 1 - \frac{g^2}{p_\theta^2} \tag{38}$$

$$E = \frac{g\left(\frac{p_\theta^2c^2}{g^2} - 1\right)}{a(1-\epsilon^2)} \tag{39}$$

and

$$\left(E^2 + \frac{g}{a(1-\epsilon^2)}q\right)^2 = p_\theta^2c^2\frac{1}{(a(1-\epsilon^2))^2}(1+\epsilon^2\omega^2) + m_e^2c^4. \tag{40}$$

Inserting $E$ to the third equation gives

$$\left(\frac{p_\theta^2c^2}{g}\right)^2 = p_\theta^2c^2(1+\epsilon^2\omega^2) + m_e^2c^4(a(1-\epsilon^2))^2. \tag{41}$$

Inserting $\omega^2$ simplifies the equation to

$$m_e^2c^4(a(1-\epsilon^2)^2 = g^2\left(\frac{p_\theta^2c^2}{g^2} - 1\right)\left(\frac{p_\theta^2c^2}{g^2} - \epsilon^2\right). \tag{42}$$

Inserting this result to the equation for $E$ gives

$$\frac{E}{m_e c^2} = \left(\sqrt{1 - \frac{g^2}{p_\theta^2 c^2}}\right)\left(\sqrt{1 - \epsilon^2 \frac{g^2}{p_\theta^2 c^2}}\right)^{-1}. \tag{43}$$

In order to go further we need the quantization rules of Sommerfeld's atomic theory.

The Wilson-Sommerfeld quantization rules are

$$\int_0^{2\pi} p_\theta d\theta = n_\theta h \tag{44}$$

and

$$\int_{r_{min}}^{r_{max}} p_r dr = n_r h. \tag{45}$$

The first quantization rule is simply $p_\theta = n_\theta \hbar$ as $p_\theta$ is constant. This quantum number is called the azimuthal quantum number in Sommerfeld's model and he introduced this quantum number, but it is not $l$ in Quantum Mechanics. It is basically $n_\theta = l + 1$. The angular momentum of a circle is not zero, therefore $n_\theta$ starts from one and reaches $n$, the principal quantum number. The second quantum number $n_r$ satisfies $n = n_r + n_\theta$ in Sommerfeld's model.

The integral in the second quantization rule can be calculated as follows.

$$p_r = p_\theta \frac{1}{r^2}\frac{dr}{d\theta} \qquad \rightarrow \qquad dr = \frac{r^2}{p_\theta} p_r d\theta \tag{46}$$

$$p_r dr = \left(p_\theta \frac{1}{r^2}\frac{dr}{d\theta}\right)\left(\frac{r^2}{p_\theta} p_r d\theta\right) = p_r \frac{dr}{d\theta} d\theta \tag{47}$$

$$= \left(p_\theta \frac{1}{r^2}\frac{dr}{d\theta}\right)\frac{dr}{d\theta} d\theta = p_\theta \frac{1}{r^2}\left(\frac{dr}{d\theta}\right)^2 d\theta \tag{48}$$

$$\int_{r_{min}}^{r_{max}} p_r dr = \int_0^{2\pi/\omega} p_\theta \frac{1}{r^2}\left(\frac{dr}{d\theta}\right)^2 d\theta \tag{49}$$

$$= \int_0^{2\pi/\omega} p_\theta \omega^2 \frac{\epsilon^2 \sin^2(\omega\theta)}{(1 + \epsilon\cos(\omega\theta))^2} d\theta \tag{50}$$

$$= p_\theta \omega \int_0^{2\pi} \frac{\epsilon^2 \sin^2(\phi)}{(1 + \epsilon\cos(\phi))^2} d\phi \tag{51}$$

$$= p_\theta \omega \left(-2\pi + \int_0^{2\pi} \frac{d\phi}{(1 + \epsilon\cos(\phi))^2}\right) \tag{52}$$

where we made integration by parts. The remaining integral is solved by Weierstrass's substition $t = \tan(\phi/2)$

$$\int \frac{d\phi}{(1+\epsilon\cos(\phi))^2} = \frac{2}{\sqrt{1-\epsilon^2}} \arctan\left(\frac{\sqrt{1-\epsilon}}{\sqrt{1+\epsilon}} \tan\left(\frac{\phi}{2}\right)\right). \tag{53}$$

The result is

$$\int_{r_{min}}^{r_{max}} p_r dr = p_\theta \omega 2\pi \left(\frac{1}{\sqrt{1-\epsilon^2}}\right) = n_r h. \tag{54}$$

Inserting $p_\theta = n_\theta \hbar$ gives the quantization rule:

$$\frac{1}{\sqrt{1-\epsilon^2}} - 1 = \frac{n_r}{\omega n_\theta}. \tag{55}$$

Inserting the equations:

$$g = \alpha c \hbar \tag{56}$$

$$p_\theta = n_\theta \hbar \tag{57}$$

$$n = n_r + n_\theta \tag{58}$$

$$\omega n_\theta = \sqrt{n_\theta^2 - \alpha^2} = n_\theta \left(1 - \frac{1}{2}\frac{\alpha^2}{n_\theta^2} - \frac{1}{8}\frac{\alpha^4}{n_\theta^4}\right) + O(\alpha^6) \tag{59}$$

into

$$\epsilon^2 = 1 - \frac{\omega^2 n_\theta^2}{(\omega n_\theta + n_r)^2} \tag{60}$$

gives after some calculation

$$\epsilon^2 = 1 - \frac{n_\theta^2}{n^2} + \alpha^2 \left(\frac{1}{n^2} - \frac{n_\theta}{n^3}\right) + O(\alpha^4). \tag{61}$$

Expanding the formula

$$\frac{E}{m_e c^2} = \left(\sqrt{1 - \frac{g^2}{p_\theta^2 c^2}}\right) \left(\sqrt{1 - \epsilon^2 \frac{g^2}{p_\theta^2 c^2}}\right)^{-1} \tag{62}$$

gives

$$\frac{E}{m_e c^2} = 1 - \frac{\alpha^2}{2n_\theta^2} + \frac{\alpha^2}{2n_\theta^2}\epsilon^2 - \frac{\alpha^4}{8n_\theta^4}\left(1 + 2\epsilon^2 - 3\epsilon^3\right) + O(\alpha^6). \tag{63}$$

Inserting the power series of $\epsilon^2$ gives Sommerfeld's fine structure spectrum formula

$$\frac{E}{m_e c^2} = 1 - \frac{\alpha^2}{2n^2} - \frac{\alpha^4}{8n_\theta n^4}\left(4n_r + n_\theta\right) + O(\alpha^6). \tag{64}$$

which can be expressed as

$$\frac{E}{m_e c^2} = 1 - \frac{\alpha^2}{2n^2} - \frac{\alpha^4}{8n_\theta n^4}\left(4n - 3n_\theta\right) + O(\alpha^6). \tag{65}$$

This is the correct formula, apart from lacking the spin.

## 3. Discussion

In order to get Sommerfeld's (correct) fine structure spectrum formula, the series expression for $\epsilon^2$ in $O(\alpha^4)$ must have all four terms in (61) correct. If the Wilson-Smmerfeld quantization rules are incorrect and there is nothing true in elliptic orbits of electrons, this is a remarkable coincidence. Free electrons move as particles along definite orbits and if there is an electromagnetic field, they change directions just like charged masses. There is no reason why a similar behavior would not continue to a very small length scale. What is true is that in small length scales there is quantization, but it can be described with quantization rules. The approach in Quantum Mechanics is inherently much more questionable. For instance, when there are two operators A and B and we calculate the expectation value of A+B by ranging over all wavefunctions $\Psi$ in $< \Psi|A + B|\Psi >$, the eigenvectors of $A + B$ are usually not the eigenvectors of either $A$ or $B$. Therefore calculating

$$< \Psi|A + B|\Psi >=< \Psi|A|\Psi > + < \Psi|B|\Psi > \tag{66}$$

does not give the eigenvalues for the operators $A + B$, $A$ and $B$ because $\Psi$ is the same. We do not get

$$ab = a + b \tag{67}$$

where $a$ is an eigenvalue of $A$, $b$ is an eigenvalue of $B$ and $ab$ is an eigenvalue of $A + B$. Ýet in the Quantum Mechanical explanation of the Zeeman effect there is an operator $A = \mathbf{J^2} - \mathbf{L^2} + \mathbf{S^2}$ and one takes the expectation value of this operator $< \Psi|A|\Psi >$. The expectation value seems to be the sum of eigenvalues of these operators, $\hbar^2(j(j + 1) - l(l + 1) + m_s(m_s + 1))$. It should not be so.

The role of the relativity theory in the derivation of Sommerfeld's formula is worth commenting as the fine structure is often proposed as verification of the relativity theory.

For S-orbits $n_\theta = 1$ ($n_\theta = l + 1$, the azimuthal quantum number in Quantum Mechanics), the orbits are circles and the velocity of the electron is $v_n = v_0/n$ where $v_0$ is the velocity of the electron on an orbit with Bohr's radius. Sommerfeld defined the fine structure constant $\alpha$ as $\alpha = v_0/c$. Sommerfeld's fine structure spectrum formula gives for S-orbits

$$E = m_e c^2 - \frac{1}{2} m_e \left(\frac{v_n}{c}\right)^2 \left(1 + \frac{3}{4}\left(\frac{v_n}{c}\right)^2\right) + O\left(\left(\frac{v_n}{c}\right)^6\right). \tag{68}$$

This is exactly the relativistic correction that would come to the kinetic energy on the S-orbit, apart of a sign

$$\sqrt{(\gamma m_e v_n)^2 c^2 + m_e^2 c^4} - m_e c^2 = \frac{1}{2} m_e \left(\frac{v_n}{c}\right)^2 \left(1 + \frac{3}{4}\left(\frac{v_n}{c}\right)^2\right) + O\left(\left(\frac{v_n}{c}\right)^6\right). \tag{69}$$

It may look like a verification of the relativistic energy formula, but the relativistic kinetic energy formula is proven incorrect both in theory and by measurements. See [2][3] and the following figure 1 from [2].

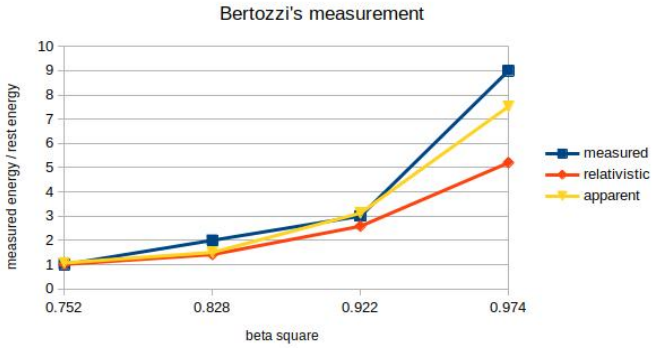


Figure 1. The figure plots $E_k/m_ec^2$ (measured), $0.5\gamma^{1.5}m_ev^2$ (kinetic energy of the apparent mass) and $(\gamma-1)m_e$ (relativistic kinetic energy) as an function of $v^2/c^2=\beta^2$. The y-axis gives the ratio of energy and the rest energy of an electron. This figure shows that $T=\sqrt{p^2c^2+m_0^2c^4}-m_0c^2=(\gamma-1)m_0c^2$ is too small and the correct energy is about $(1/2)\gamma^{1.5}m_ov^2$.

It is correct and necessary to use an apparent mass because early measurements by physicists (like Lorentz) did show that electrons have apparent mass in an electromagnetic field, but if is fine to replace the apparent kinetic energy (which is not known and depends on the situation) with the relativistic kinetic energy in the fine structure spectrum case. This is because $v_0=\alpha c$ and $\alpha$ is small, about 0.007. The more correct (but not perfect) kinetic energy formula $(1/2)\gamma^{1.5}m_ov^2$ gives exactly the same first order approximation as the relativistic kinetic energy. Sommerfeld does not have an error here, but one can conclude that the good match of Sommerfeld's fine structure spectrum with measurements is not a verification of the relativistic kinetic energy formula.

Next, a small comment on the Quantum Mechanical derivation of the fine structure spectrum formula, see [4]. We saw that for S-orbits the energy $E$ can indeed be understood as a relativistic correction. But when $n_\theta>0$ the orbits are not circles in Sommerfeld's model and there are no orbits in the Quantum Mechanical model. There is no reason to consider the first term in the fine structure spectrum formula as a relativistic correction. In the derivation of Sommerfeld's formula the terms come from quantization rules applied to elliptic orbits and there is no use of relativity theory at all, $p_r$ and $p_\theta$ are never evaluated in a way that could show if the mass in them is $\gamma m_e$. It can be the apparent mass, which is very closely the same.

Finally, let me make a small comment on inclusion of spin in Sommerfeld's formula. Sommerfeld was never satisfied with his efforts to include spin and to explain the Zeeman effect. Both situations are rather similar. In the spin effect

to the fine structure spectrum formula, the magnetic field is that of the proton. We can assume in Sommerfeld's model that a proton is a magnetic dipole and electrons orbit, like in a planetary system, on a plane that is orthogonal to the axis of this dipole. Then the magnetic field $\vec{B}$ can be taken as being on the z-direction and the plane where electrons circulate is the (x,y)-plane. If the orbit is an ellipse, the velocity vector of an electron has a radial and angular component, $\vec{v}_r$, $\vec{v}_\phi$. The force $\vec{F}$ from the magnetic field is $\vec{v} \times \vec{B}$ has a radial and angular component. It seems that in Quantum Mechanics the change of energy levels caused by a magnetic field is calculated from operators $\mathbf{L}$ and $\mathbf{B}$ as $E = (q/m)\mathbf{L} \cdot \mathbf{B}$, which in a vector model corresponds to $E = (q/m)\vec{L} \cdot \vec{B}$. This is work done by a force in the radial direction causing the orbit to move in the radial direction. But the orbit does not move in the radial directions. We know it because electrons circulating the nucleus do not radiate even though the orbit is curved. The orbit cannot get gradually smaller. Only by an emission or absorbtion of a photon the quantized orbit can change. Therefore the radial force cannot do work and as it does not do work, energy from the field does not add to the energy of the atom/electron. There is also the angular component of the force. It also cannot do work because the angular momentum is conserved.

Therefore my opinion is that the effect of a magnetic field, both in the spin in the fine structure spectrum formula and in the Zeeman effect, is not that the field directly makes work. The field gives a force that either increases or decreases the Coulomb force. When the Coulomb force is increased or decreased, it changes the orbits that the electrons can have. These orbits are quantized by Wilson-Somerfeld quantization rules. Therefore the effect of a magnetic force is that it changes the rules of counting quantum numbers.

In the case of the spin in the fine structure spectrum formula, this change of rules could be that $n = n_r + n_\theta$ is not always true. If the electron spin is one way, the rule is $n = n_r + n_\theta$, while if the spin is the other way, the rule is e.g. $n = 1 + n_r + n_\theta$.

Like Sommerfeld, I am not satisfied with my efforts to model the spin issue and the Zeeman effect in a semiclassical model, at least so far, but I suggest looking for a solution that changes the quantization rules, mainly how they are summed. There naturally is a need for the magnetic quantum number $m_l$, and how to put it to the model? But these issues should not cause a rejection of Bohr-Sommerfeld type semiclassical models. I find the derivation of Sommerfeld's formula much more convincing than the derivation in Quantum Mechanics. In Quantum Mechanics, like in the Relativity Theory, I mostly see errors and contradictions. Surprisingly, Sommerfeld's formula was correctly calculated and makes sense.

## 4. References

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