KLEIN-GORDON EQUATION WITH COULOMB POTENTIAL - HYPERGEOMETRIC FUNCTIONS AND NUMERICAL SOLUTIONS

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Reference: W. Greiner: *Relativistic Quantum Mechanics (Wave Equations)*; 3rd Edition, Springer-Verlag (2000); Section 1.9, Exercise 1.11.

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If we follow Greiner's solution of the Klein-Gordon equation for a particle in a Coulomb potential, we arrive at a radial function $u(r)$ given by

$$u(r) = \frac{R(r)}{r} \tag{1}$$

where the auxiliary radial function R is given by

$$R(\rho) = N\rho^{\mu+1/2}e^{-\rho/2}f(\rho) \tag{2}$$

Here, some parameters are used to simplify the notation:

$$\beta \equiv 2\frac{\sqrt{m_0^2c^4-\varepsilon^2}}{\hbar c} \tag{3}$$

$$\rho \equiv \beta r \tag{4}$$

$$\mu \equiv \sqrt{\left(l+\frac{1}{2}\right)^2 - Z^2\alpha^2} \tag{5}$$

$$\lambda \equiv \frac{2Z\alpha\varepsilon}{\hbar c\beta} \tag{6}$$

where ε is the energy parameter in the stationary state. Of these parameters, ρ, μ and λ are all dimensionless. With these definitions, the auxiliary radial function $R(\rho)$ satisfies the differential equation

$$\left(\frac{d^2}{d\rho^2} - \frac{\mu^2-\frac{1}{4}}{\rho^2} + \frac{\lambda}{\rho} - \frac{1}{4}\right)R_l(\rho) = 0 \tag{7}$$

where the subscript l indicates the angular momentum quantum number that appears in the angular part of the solution.

I tried solving this ODE numerically using Maple, but the singularity at $\rho = 0$ proved too much for it to handle. As a result, we can continue with

Greiner's solution, in which he looks at the asymptotic nature of the solution for $\rho \to 0$ and $\rho \to \infty$. This analysis is similar to that done for the hydrogen atom in the Schrödinger equation. The result is that we can write R as

$$R(\rho) = N\rho^{\mu+\frac{1}{2}} e^{-\rho/2} f(\rho) \tag{8}$$

where $f(\rho)$ satisfies the ODE

$$\frac{d^2 f}{d\rho^2} + \left(\frac{2\mu+1}{\rho} - 1\right)\frac{df}{d\rho} - \frac{\mu+\frac{1}{2}-\lambda}{\rho} f = 0 \tag{9}$$

We can use a series solution, also analogous to the hydrogen atom case. We try

$$f(\rho) = \sum_{n=0}^{\infty} a_n \rho^n \tag{10}$$

and upon substituting this back into 9 we find that the coefficients are determined by the recursion relation

$$a_m = \frac{a+m-1}{m(d+m-1)} a_{m-1} \tag{11}$$

with the constants d and a defined as

$$a \equiv \mu + \frac{1}{2} - \lambda \tag{12}$$

$$d \equiv 2\mu + 1 \tag{13}$$

The recursion relation gives a_m in single steps, so we need to specify only the initial term a_0 to get things started. The function thus becomes

Greiner uses the symbol c for what I've called d, but this can be confused with the speed of light, so I've used d instead.

$$f(\rho) = a_0\left(1 + \frac{a}{d}\rho + \frac{a(a+1)}{d(d+1)}\frac{\rho^2}{2!} + \ldots\right) \tag{14}$$

$$= a_0 \sum_{m=0}^{\infty} \frac{a^{(m)}}{d^{(m)}} \frac{\rho^m}{m!} \tag{15}$$

The notation $a^{(m)}$ denotes a *rising factorial* which is defined as

$$a^{(m)} \equiv \prod_{k=1}^{m} (a+k-1) \tag{16}$$

$$= a(a+1)\ldots(a+m-1) \tag{17}$$

Greiner calls this a 'generalized faculty function' and uses the notation $(a)_m$ which doesn't appear to be standard.

The function defined by 15 is a *confluent hypergeometric function* and is written as ${}_1F_1(a,d;\rho)$. As with the series solution for hydrogen, ${}_1F_1$ blows up as $\rho\to\infty$, so we must require that the series terminates at some m. This will happen if $a=-n'$ for some integer n' and imposing this condition leads, via 12, to a quantization condition on the energy ε. Doing the algebra gives us

$$\varepsilon_{nl}=\pm m_0c^2\left[1+\frac{Z^2\alpha^2}{\left(n'+\frac{1}{2}+\sqrt{\left(l+\frac{1}{2}\right)^2-Z^2\alpha^2}\right)^2}\right]^{-1/2} \tag{18}$$

At this point, Greiner says we must take the minus sign because in the case of zero electric field (which Greiner says is the case $Z\alpha\to\infty$, but it would seem to me that this should be $Z\alpha\to 0$, since zero field would mean that we have no charges present, so $Z=0$) we need $\varepsilon<0$ for a negatively charged particle. This appears to arise from the free-particle solution we found earlier, where

$$\psi_{\pm}=A_{(\pm)}e^{i\left(\mathbf{p}\cdot\mathbf{x}\mp\left|E_p\right|t\right)/\hbar} \tag{19}$$

If we take $Z=0$, then

$$\varepsilon=\pm m_0c^2 \tag{20}$$

which does make sense for a free particle. Taking $Z\to\infty$ gives an imaginary number for the square root in the denominator, which doesn't make sense for an energy.

Greiner then states that the 'energy itself' is given by

$$E_{nl}=m_0c^2\left[1+\frac{Z^2\alpha^2}{\left(n'+\frac{1}{2}+\sqrt{\left(l+\frac{1}{2}\right)^2-Z^2\alpha^2}\right)^2}\right]^{-1/2} \tag{21}$$

that is, just the positive root from 18. He also says that it is the integral of the 00 component of the energy-momentum tensor, which he works out in detail in his Exercise 1.12. Given the complexity of T_{00} (see Greiner's eqn (8) in Exercise 1.12 - I don't want to write the whole thing out here!), evaluating $\int T_{00}d^3x$ doesn't look particularly easy, so we'll take his word for it.

In any case, the important thing to note from 21 is the quantity in brackets is always greater than 1, so raising it to the power of $-\frac{1}{2}$ gives a value between 0 and 1. Thus E_{nl} is always reduced from the free particle energy of m_0c^2, and the amount by which it is reduced is the binding energy E_b, so we have

$$E_b \equiv E_{nl} - m_0c^2 \tag{22}$$

Defining the principal quantum number as

$$n \equiv n' + l + 1 \tag{23}$$

we get

$$E_{nl} = m_0c^2 \left[1 + \frac{Z^2\alpha^2}{\left(n - l - \frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 - Z^2\alpha^2} \right)^2} \right]^{-1/2} \tag{24}$$

We can expand this in a Taylor series in Z about $Z = 0$ (which I checked using Maple) and we get

$$E_{nl} = m_0c^2 \left[1 - \frac{Z^2\alpha^2}{2n^2} - \frac{Z^4\alpha^4}{n^4} \left(\frac{n}{2l+1} - \frac{3}{8} \right) + \ldots \right] \tag{25}$$

Note that the numerator in the last term should be n and not a as given in Greiner.

The second term works out to

$$-m_0c^2 \frac{Z^2\alpha^2}{2n^2} = -m_0c^2 \frac{Z^2}{2n^2} \frac{e^4}{\hbar^2 c^2} \tag{26}$$

$$= -\frac{Z^2 m_0 e^4}{2n^2\hbar^2} \tag{27}$$

This is the formula for the Bohr energy levels for a single electron around a nucleus with charge Ze. The last (and higher order) terms in 25 are the relativistic corrections arising from using the Klein-Gordon equation instead of the non-relativistic Schrödginer equation.

The final form for the auxiliary radial function $R(\rho)$ is (using 12)

$$R(\rho) = N'\rho^{\mu+\frac{1}{2}} e^{-\rho/2} {}_1F_1(a, d; \rho) \tag{28}$$

$$= N'\rho^{\mu+\frac{1}{2}} e^{-\rho/2} {}_1F_1\left(\mu + \frac{1}{2} - \lambda, 2\mu + 1; \rho\right) \tag{29}$$

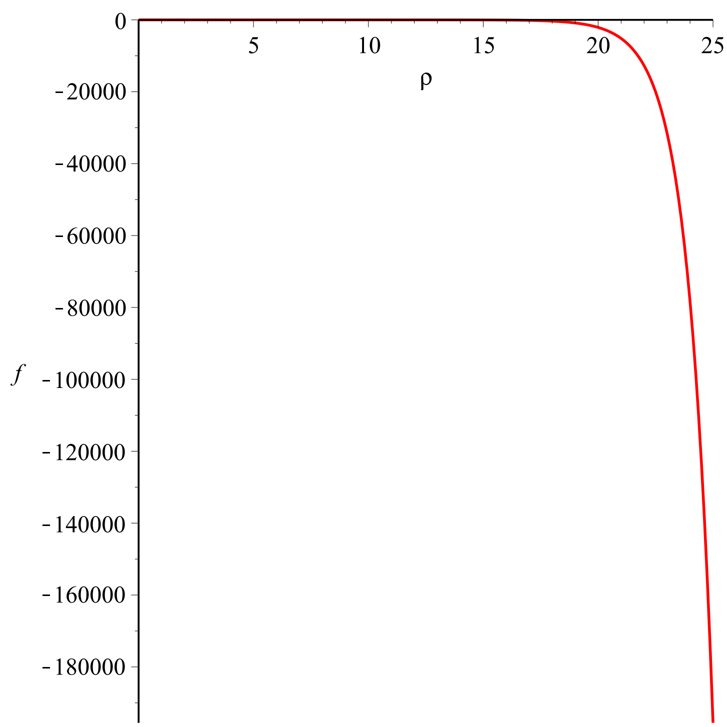
$$\equiv N' W_{\lambda,\mu}(\rho) \tag{30}$$

where $W_{\lambda,\mu}(\rho)$ is a *Whittaker function,* and N' is a normalization constant.

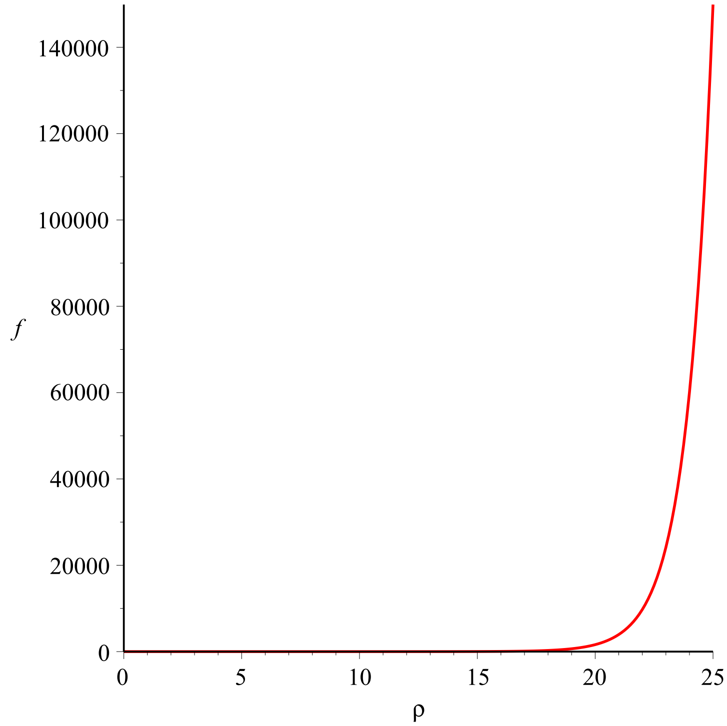
Finally, it's interesting to see how we can solve this system numerically, using the 'wag the dog' method that we used earlier to solve some non-relativistic problems numerically. In this case, we can use the ODE 9, and cheat a bit by using some of the properties of the solution. This ODE also has a singularity at $\rho = 0$, but in solving the system in Maple, we can start the integration at a value of ρ slightly greater than 0. If we choose ε to be one of the energy eigenvalues, then we should find that f flips over from blowing up on the negative side to the positive side as we vary ε across this value. In Greiner's table of results in Exercise 1.11, he gives the binding energy of a pion around a nucleus with charge $Z = 10$ in an $l = 0$ state as -0.374 MeV. The rest energy of a pion is 139.577 MeV, so the energy eigenvalue is

$$E_{10} = 139.577 - 0.374 = 139.203 \text{ MeV} \tag{31}$$

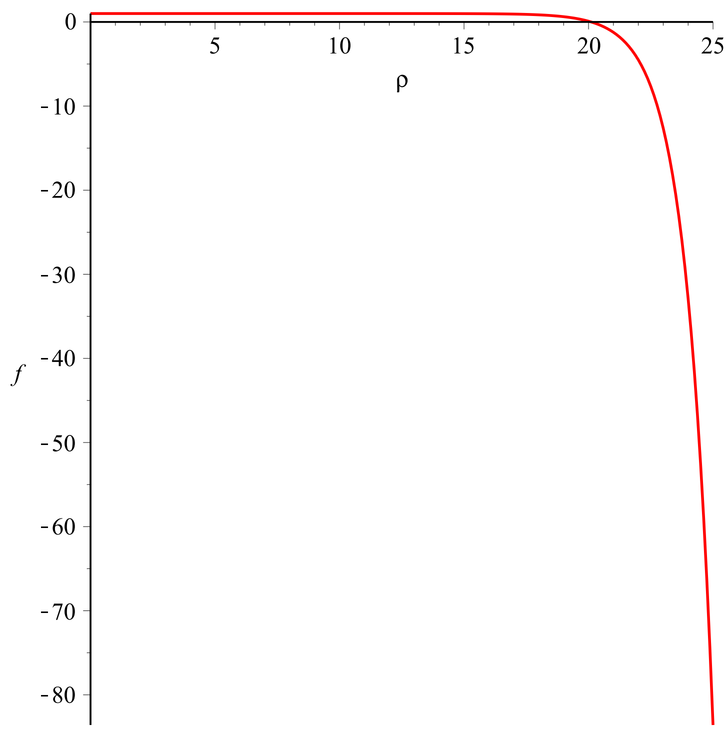
If we try 139.204, we find the function blows up on the negative side:



For 139.202, it blows up on the other side:



By trying values between these two points, we can narrow down the eigenvalue. For a value of 139.2028655 we get:



Although this still blows up, note that the scale on the vertical axis is much smaller than on the preceding two graphs, so we're getting closer to the actual value. The binding energy at this point is

$$E_{b,10} = -0.3741345 \text{ MeV} \tag{32}$$

It's also worth noting that to solve this equation, we don't need to specify the value of n, the principal quantum number. In fact, once we find ε by 'wagging the dog', we would then work backwards to determine n from ε using 24.

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