KLEIN-GORDON EQUATION WITH EXPONENTIAL POTENTIAL

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Reference: W. Greiner: *Relativistic Quantum Mechanics (Wave Equations)*; 3rd Edition, Springer-Verlag (2000); Section 1.11, Exercise 1.15.

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We'll have a look at the Klein-Gordon equation with an exponential potential of form

$$V(r) = -Z\alpha e^{-r/a} \tag{1}$$

Here Z is the nuclear charge number (charge in units of e) and

$$\alpha = \frac{m_0 c^2 e^2}{\hbar c} \tag{2}$$

Greiner says that if we use natural units then $m_0 = c = \hbar = 1$ and α is 'equivalent' to the fine structure constant, which is the usual meaning of α. However, as we've been using explicit values for these constants in previous posts, we'll continue to use $e^2/\hbar c$ as the fine structure constant (with value $\frac{1}{137}$) and multiply by the rest energy $m_0 c^2$ of the particle concerned (usually a pion, where $m_0 c^2 = 139.57$ MeV).

The Klein-Gordon equation for a spherically symmetric potential reduces to the radial equation

$$\left[-\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{l(l+1)}{r^2}\right]u(r) = \frac{(\varepsilon - V)^2 - m_0^2 c^4}{\hbar^2 c^2}u(r) \tag{3}$$

This is solved by defining

$$u(r) \equiv \frac{R(r)}{r} \tag{4}$$

and then dealing with the ODE for R, which is

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2\right]R(r) = 0 \tag{5}$$

with

$$k^2 \equiv \frac{(\varepsilon - V)^2 - m_0^2 c^4}{\hbar^2 c^2} \tag{6}$$

If we consider s states, where $l = 0$, then the ODE becomes

$$\left[\frac{d^2}{dr^2} + k^2\right] R(r) = 0 \tag{7}$$

With $V(r)$ given by 1, we can introduce a separation ansatz with

$$R(r) = e^{r/2a} w(t) \tag{8}$$

with t defined by

$$t \equiv 2iZ\alpha \frac{a}{\hbar c} e^{-r/a} \tag{9}$$

To transform 7 we need to work out the second derivative using 8 and convert the ODE to an ODE in t. For this purpose, we'll use the shortand notation

$$t = Ae^{-r/a} \tag{10}$$

where

$$A \equiv 2iZ\alpha \frac{a}{\hbar c} \tag{11}$$

We have

$$\begin{aligned}
\frac{dR}{dr} &= \frac{1}{2a} e^{r/2a} w(t) + e^{r/2a} \frac{dw}{dt} \frac{dt}{dr} && (12)\\
&= \frac{1}{2a} e^{r/2a} w(t) - e^{r/2a} \frac{A}{a} e^{-r/a} \frac{dw}{dt} && (13)\\
&= \frac{e^{r/2a}}{a} \left[\frac{1}{2} w(t) - Ae^{-r/a} \frac{dw}{dt}\right] && (14)\\
\frac{d^2R}{dr^2} &= \frac{e^{r/2a}}{a} \left\{ \frac{1}{2a} \left[\frac{1}{2} w(t) - Ae^{-r/a} \frac{dw}{dt}\right] - \right. && (15)\\
&\quad \left. \frac{1}{2} \frac{dw}{dt} \frac{A}{a} e^{-r/a} + \frac{A}{a} e^{-r/a} \frac{dw}{dt} + \frac{A^2}{a} e^{-2r/a} \frac{d^2w}{dt^2} \right\} && (16)\\
&= \frac{e^{r/2a}}{a^2} \left[t^2 \frac{d^2w}{dt^2} + \frac{w}{4}\right] && (17)
\end{aligned}$$

Expanding k^2 from 6 with 1 we have

$$k^2R = \frac{\left(\varepsilon + Z\alpha e^{-r/a}\right)^2 - m_0^2c^4}{\hbar^2c^2} e^{r/2a} w(t) \tag{18}$$

$$= \left[\frac{\varepsilon^2 - m_0^2c^4}{\hbar^2c^2} + \frac{2\varepsilon Z\alpha e^{-r/a}}{\hbar^2c^2} + \frac{Z^2\alpha^2 e^{-2r/a}}{\hbar^2c^2}\right] e^{r/2a} w(t) \tag{19}$$

$$= \left[-p^2 + \frac{\varepsilon t}{\hbar cai} - \frac{t^2}{4a^2}\right] e^{r/2a} w(t) \tag{20}$$

where

$$p^2 \equiv \frac{m_0^2c^4 - \varepsilon^2}{\hbar^2c^2} \tag{21}$$

Cancelling off the $e^{r/2a}$ and collecting terms, we have

In Greiner's eqn (7) he misses the 2 exponent on the $\hbar$ in the denominator.

$$\frac{t^2}{a^2}\frac{d^2w}{dt^2} + \left(\frac{1}{4a^2} - p^2 + \frac{\varepsilon t}{\hbar cai} - \frac{t^2}{4a^2}\right) w = 0 \tag{22}$$

Finally, multiplying through by a^2/t^2 we have

$$\frac{d^2w}{dt^2} + \left(-\frac{1}{4} - \frac{i\varepsilon a}{\hbar ct} + \frac{\frac{1}{4} - p^2a^2}{t^2}\right) w = 0 \tag{23}$$

This ODE has as its solutions the Whittaker functions (which we met earlier while looking at the Coulomb potential), so the solution is

$$w(t) = NW_{\lambda,\mu}(t) \tag{24}$$

$$= Ne^{-t/2}t^{\mu+\frac{1}{2}} {}_1F_1\left(\frac{1}{2} + \mu - \lambda, 1 + 2\mu; t\right) \tag{25}$$

where ${}_1F_1$ is the confluent hypergeometric function. The radial function then becomes

$$u(r) = \frac{R(r)}{r} \tag{26}$$

$$= N\frac{e^{r/2a}}{r} W_{\lambda,\mu}\left(2iZ\alpha\frac{a}{\hbar c}e^{-r/a}\right) \tag{27}$$

At this point, Greiner claims that in order for the radial function to be normalizable, we must have $R(r) = 0$ at $r = 0$. I'm not sure where he gets this condition from, since even though the radial function $u(r) = R(r)/r$ would have a singularity at $r = 0$ if $R(0) \neq 0$, when we normalize u we square it and multiply by the radial integration element r^2dr, so the singularity would cancel out. It would seem to be more important to ensure that R goes to zero for large r, so I'm confused.

Anyway, if we accept Greiner's statement, then the condition becomes

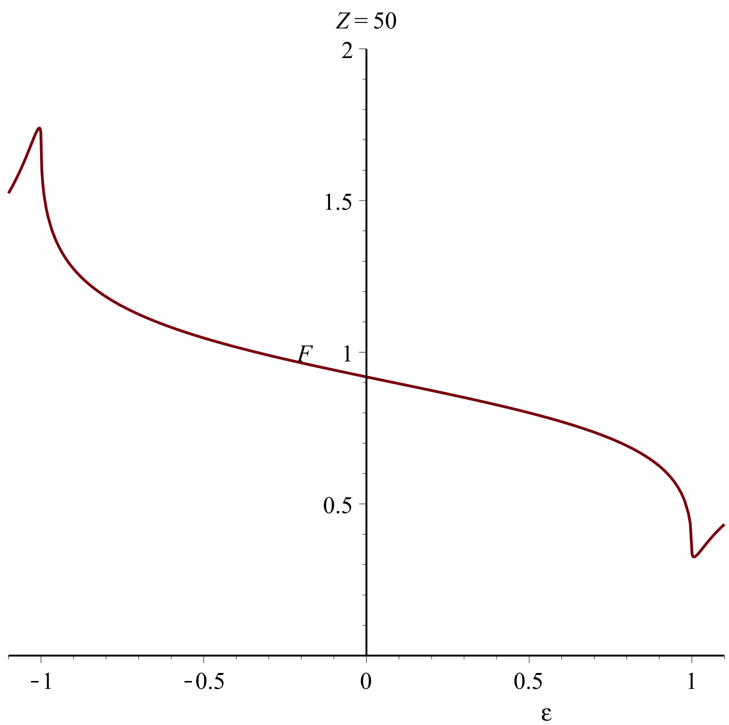
$$W_{\lambda,\mu}\left(2iZ\alpha\frac{a}{\hbar c}\right)=0 \tag{28}$$

which, from 25 gives the condition

$${}_1F_1\left(\frac{1}{2}+\mu-\lambda,1+2\mu;2iZ\alpha\frac{a}{\hbar c}\right)=0 \tag{29}$$

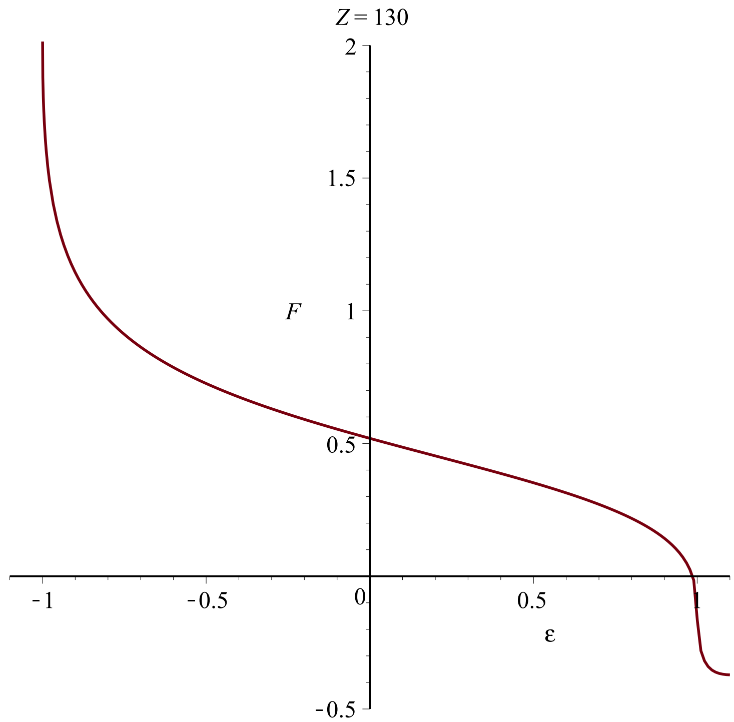
Maple's 'hypergeom' function gives values for ${}_1F_1$ and we can use 'fsolve' to find the value of ε that solves 29. However, it's more revealing to use a graphical method. As usual, we would expect that for small values of Z, we would get fewer (or possibly no) bound states, and we'd expect that as Z increases, the lowest energy bound state would get lower, and that more bound states might appear above this lowest state.

If we try $Z=50$ and plot ${}_1F_1$ versus ε/m_0c^2, we see that ${}_1F_1$ has no zeros for energies between $-m_0c^2$ and $+m_0c^2$ (a range of -1 to $+1$ on the ε (horizontal) axis).

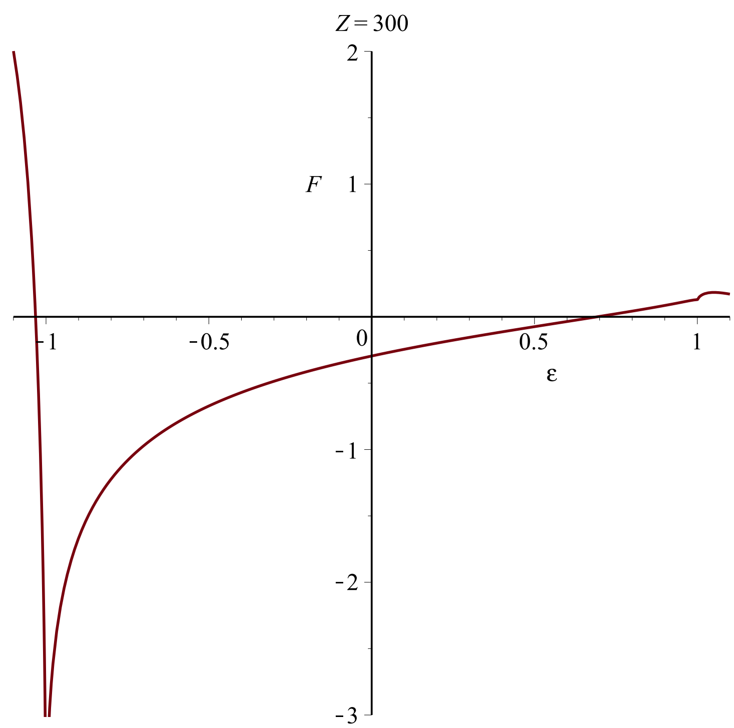


Plots show the real part of ${}_1F_1$, but at the point where ${}_1F_1$ crosses the horizontal axis, both real and imaginary parts are zero. At intermediate points, both real and imaginary parts are in general non-zero.

At $Z=130$, there is a zero very near $\varepsilon=1$ (the actual value is $\varepsilon=0.986m_0c^2$).



For $Z = 300$, the energy has dropped to $\varepsilon = 0.692 m_0 c^2$.



For $Z = 600$, the ground state has dropped to $\varepsilon = -0.276 m_0 c^2$ and a second zero appears near $\varepsilon = 0.8 m_0 c^2$.