

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

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

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

$$\alpha = \frac{m_0 c^2 e^2}{\hbar c} \quad (2)$$

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

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

This is solved by defining

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

and then dealing with the ODE for R , which is

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

with

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

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

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

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

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

with t defined by

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

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 shorthand notation

$$t = Ae^{-r/a} \quad (10)$$

where

$$A \equiv 2iZ\alpha \frac{a}{\hbar c} \quad (11)$$

We have

$$\frac{dR}{dr} = \frac{1}{2a} e^{r/2a} w(t) + e^{r/2a} \frac{dw}{dt} \frac{dt}{dr} \quad (12)$$

$$= \frac{1}{2a} e^{r/2a} w(t) - e^{r/2a} \frac{A}{a} e^{-r/a} \frac{dw}{dt} \quad (13)$$

$$= \frac{e^{r/2a}}{a} \left[\frac{1}{2} w(t) - Ae^{-r/a} \frac{dw}{dt} \right] \quad (14)$$

$$\frac{d^2R}{dr^2} = \frac{e^{r/2a}}{a} \left\{ \frac{1}{2a} \left[\frac{1}{2} w(t) - Ae^{-r/a} \frac{dw}{dt} \right] - \right. \quad (15)$$

$$\left. \frac{1}{2} \frac{dw}{dt} \frac{A}{a} e^{-r/a} + \frac{A}{a} e^{-r/a} \frac{dw}{dt} + \frac{A^2}{a} e^{-2r/a} \frac{d^2w}{dt^2} \right\} \quad (16)$$

$$= \frac{e^{r/2a}}{a^2} \left[t^2 \frac{d^2w}{dt^2} + \frac{w}{4} \right] \quad (17)$$

Expanding k^2 from 6 with 1 we have

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

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

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

where

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

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

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

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

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

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

$$w(t) = N W_{\lambda, \mu}(t) \quad (24)$$

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

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

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

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

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

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

square it and multiply by the radial integration element $r^2 dr$, 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

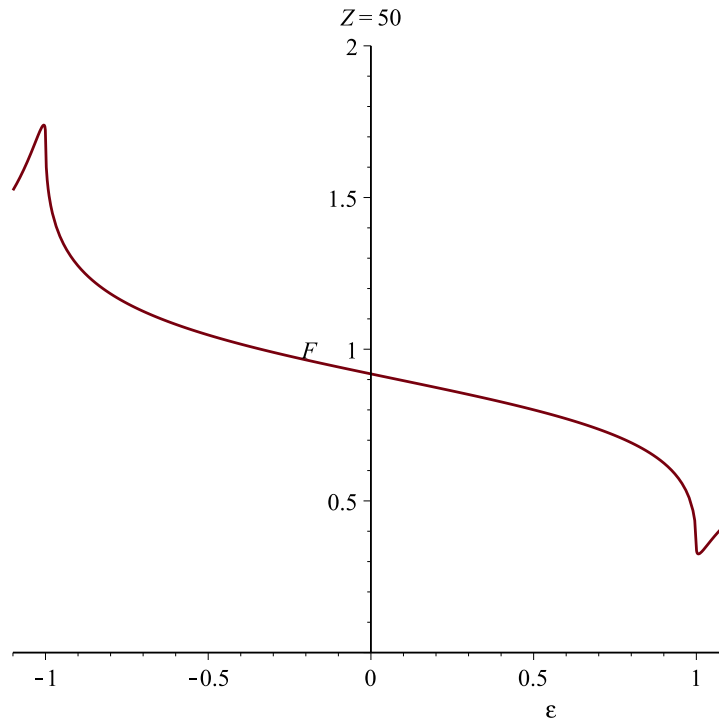
$$W_{\lambda,\mu} \left(2iZ\alpha \frac{a}{\hbar c} \right) = 0 \tag{28}$$

which, from 25 gives the condition

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

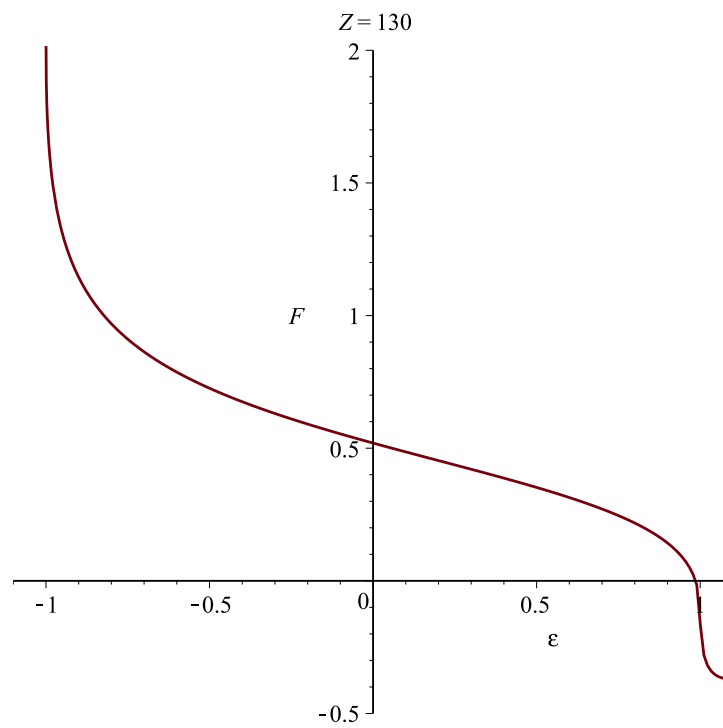
Maple's 'hypergeom' function gives values for ${}_1F_1$ and we can use 'fsolve' to find the value of ϵ that solves 29. However, it's more revealing to use a graphical method. As usual, we would expect that for small values of Z , we would get fewer (or possibly no) bound states, and we'd expect that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

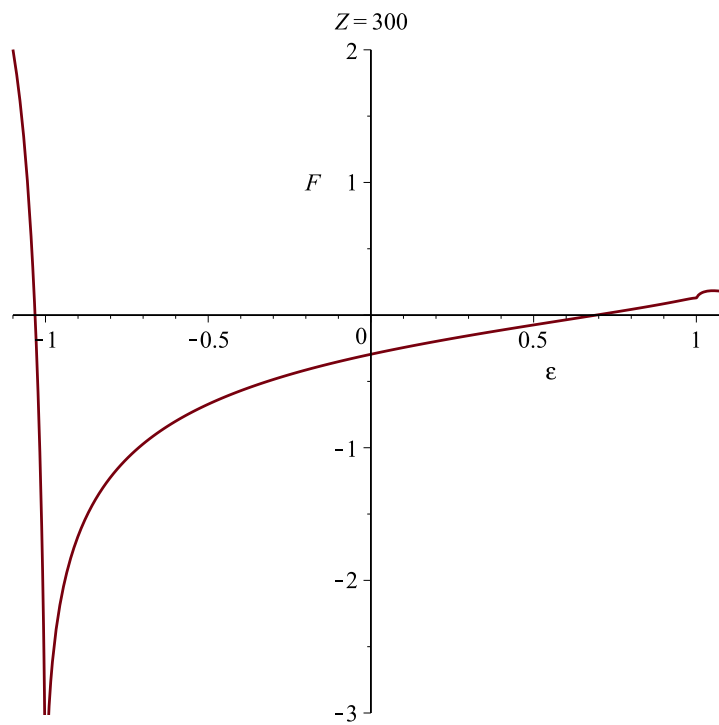


Plots show the real part of ${}_1F_1$, but at the point where ${}_1F_1$ crosses the horizontal axis, both real and imaginary parts are zero. At intermediate points, both real and imaginary parts are in general non-zero.

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



For $Z = 300$, the energy has dropped to $\epsilon = 0.692m_0c^2$.



For $Z = 600$, the ground state has dropped to $\varepsilon = -0.276m_0c^2$ and a second zero appears near $\varepsilon = 0.8m_0c^2$.

