KLEIN-GORDON EQUATION WITH FINITE SQUARE WELL

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Reference: W. Greiner: *Relativistic Quantum Mechanics (Wave Equations)*; 3rd Edition, Springer-Verlag (2000); Section 1.11, Example 1.14.

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Another example of the Klein-Gordon equation with a radially symmetric potential is the case of the finite spherical square well. The potential is given by

$$V(r)=\begin{cases}-V_0 & r\le R\\ 0 & r>R\end{cases} \tag{1}$$

We treated a similar system (although it was for an infinite spherical square well) with the Schrödinger equation earlier, and it turns out that similar equations turn up with the K-G equation. The radial K-G equation is

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

We define

$$k_i=\frac{\sqrt{(\varepsilon+V_0)^2-m_0^2c^4}}{\hbar c};\;\;\text{for } r\le R \tag{3}$$

$$k_o=\frac{\sqrt{\varepsilon^2-m_0^2c^4}}{\hbar c};\;\;\text{for } r>R \tag{4}$$

In most cases, we'd expect the well depth V_0 and the overall energy ε to be less than the rest energy m_0c^2, so in these cases, both k_i and k_o are pure imaginary numbers. Using these symbols and multiplying 2 through by $-r^2$ we get

$$\left[\frac{d}{dr}\left(r^2\frac{d}{dr}\right)-l(l+1)+k_{i,o}^2r^2\right]u(r)=0 \tag{5}$$

where we choose the subscript i or o depending on r. To eliminate $k_{i,o}$ we introduce the variable

$$\rho\equiv kr \tag{6}$$

where I'm using the generic symbol k to represent both $k_{i,o}$. Therefore

$$r = \frac{\rho}{k} \tag{7}$$

$$\frac{d}{dr} = k\frac{d}{d\rho} \tag{8}$$

$$\frac{d^2}{dr^2} = k^2\frac{d^2}{d\rho^2} \tag{9}$$

Note that ρ is also an imaginary number (since k is imaginary and r must be real). Plugging these into 5 we get

$$\left[\rho^2\frac{d^2}{d\rho^2} + 2\rho\frac{d}{d\rho} + \rho^2 - l(l+1)\right]u(\rho) = 0 \tag{10}$$

This equation is the defining ODE for spherical Bessel functions, so the general solution is

$$u(\rho) = Aj_l(\rho) + Bn_l(\rho) \tag{11}$$

where j_l is the spherical Bessel function of the first kind and n_l is the spherical Bessel function of the second kind (sometimes called a Neumann function).

For the case $r \le R$, we must exclude the Neumann functions as they blow up for $r \to 0$, so the solution is

$$u_i(\rho) = u(k_i r) = N_i j_l(k_i r) \text{ for } r \le R \tag{12}$$

where N_i is a normalization constant. It's important to note that j_l is here a function of an imaginary argument.

In the text, following Greiner's eqn (3), he writes j_l as a subscript of the normalization constant N. The j_l should be multiplied by N, not be a subscript of it.

For $r > R$, we can write the solution in terms of the spherical Hankel functions, which are just linear combinations of spherical Bessel functions. They are of two kinds, defined as

$$h_l^{(1)}(\rho) \equiv j_l(\rho) + in_l(\rho) \tag{13}$$

$$h_l^{(2)}(\rho) \equiv j_l(\rho) - in_l(\rho) \tag{14}$$

Note that $h_l^{(2)}$ is the complex conjugate of $h_l^{(1)}$ *only* if the corresponding Bessel functions are real, which won't be true in our case.

Some properties of the spherical Hankel functions can be found here (for the first kind) and here (for the second kind). It's important to note that we're dealing with *spherical* Bessel and Hankel functions here; there are other types of both functions that don't concern us here.

In our case, we're dealing with $r > R$, so we need to investigate the properties of the Hankel functions for large imaginary arguments. The asymptotic forms are

$$h_l^{(1)}(\rho) \to (-i)^{l+1} \frac{e^{i\rho}}{\rho} \tag{15}$$

$$h_l^{(2)}(\rho) \to i^{l+1} \frac{e^{-i\rho}}{\rho} \tag{16}$$

If ρ is imaginary with a positive imaginary part, then $e^{-i\rho} \to \infty$ for large ρ, while $e^{i\rho} \to 0$. Thus we must exclude $h_l^{(2)}(\rho)$ from the solution, so that for $r > R$ we have

$$u_o(\rho) = u(k_o r) = N_o h_l^{(1)}(k_o r) \tag{17}$$

where N_o is another normalization constant.

For some reason, Greiner defines another k by $k^2 = -k_o^2$, so that this k is real. However, he then makes the substitution $\rho = ikr$ in 5 and states the ODE again as 10 divided through by ρ^2 (and gets it wrong, as the second term in his eqn (6) should be $\frac{2}{\rho}\frac{du}{d\rho}$). However, his eqns (6) and (3) are essentially identical, so I don't see why he went through all this.

In any case, we now have solutions for the two regions of r, so to find the allowable energies, we require the wave function and its derivative to be continuous at $r = R$. This leads to

$$u_i(k_i R) = u_o(k_o R) \tag{18}$$

$$\frac{d}{dr}[u_i(k_i R)] = \frac{d}{dr}[u_o(k_o R)] \tag{19}$$

Dividing the second equation by the first and using 12 and 17, we get Greiner's eqn (11):

$$\frac{j_l'(k_i R)}{j_l(k_i R)} = \frac{h_l^{(1)\prime}(k_o R)}{h_l^{(1)}(k_o R)} \tag{20}$$

where the primes in the numerators indicate a derivative with respect to r.

For the case $l = 0$, we know the explicit forms of the solutions as

$$j_0(k_i r) = \frac{\sin(k_i r)}{k_i r} \tag{21}$$

$$h_0^{(1)}(k_o r) = -\frac{i}{k_o r} e^{i k_o r} \tag{22}$$

The derivatives are

$$j_0'(k_i r) = \frac{1}{k_i}\frac{k_i r\cos(k_i r) - \sin(k_i r)}{r^2} \tag{23}$$

$$h_0^{(1)}(k_o r) = -\frac{i}{k_o}\frac{ik_o r - 1}{r^2}e^{ik_o r} \tag{24}$$

The boundary condition 20 is therefore

$$\frac{j_0'(k_i R)}{j_0(k_i R)} = \frac{1}{k_i}\frac{k_i R\cos(k_i R) - \sin(k_i R)}{R^2} \times \frac{k_i R}{\sin(k_i R)} \tag{25}$$

$$= k_i \cot(k_i R) - \frac{1}{R} \tag{26}$$

$$\frac{h_0^{(1)\prime}(k_o R)}{h_0^{(1)}(k_o R)} = -\frac{i}{k_o}\frac{ik_o R - 1}{R^2}e^{ik_o R} \times \left(-\frac{k_o R}{ie^{ik_o R}}\right) \tag{27}$$

$$= ik_o - \frac{1}{R} \tag{28}$$

Setting the two sides equal gives the condition

$$k_i \cot(k_i R) = ik_o \tag{29}$$

Since k_o is imaginary, the RHS is real. The LHS is real also, as we can see by expanding the cotangent:

$$k_i \cot(k_i R) = k_i \frac{\cos(k_i R)}{\sin(k_i R)} \tag{30}$$

$$= k_i \frac{e^{ik_i R} + e^{-ik_i R}}{e^{ik_i R} - e^{-ik_i R}}\frac{2i}{2} \tag{31}$$

$$= ik_i \frac{e^{ik_i R} + e^{-ik_i R}}{e^{ik_i R} - e^{-ik_i R}} \tag{32}$$

Since k_i is imaginary, all the exponentials are real, and ik_i is also real. To find the energy levels, we therefore need to plug in the values in the expressions 3 and 4 and then solve 29 numerically for ε. This can be done by using software, or by the graphical method we used earlier for solving the finite square well in one dimension with the Schrödinger equation. Greiner gives a few examples at the end of his Example 1.14.

PINGBACKS

Pingback: Klein-Gordon equation with finite square well - numerical solution