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The Dirac equation with a δ-potential

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Abstract. An elementary treatment of the Dirac equation in the presence of a three-dimensional spherically symmetric $\delta(r - r_0)$-potential is presented. We show how to handle the matching conditions in configuration space, and discuss the occurrence of supercritical effects.

The problem of solving the Dirac equation in the presence of a δ-potential represents a curious and non-simple situation, in contrast with the equivalent problem in non-relativistic quantum mechanics, i.e. the Schrödinger equation, which is discussed in any course on quantum mechanics. This is basically related to the fact that, being the Dirac equation of first order, a singular potential, like the δ one, induces discontinuities at the level of the wavefunctions themselves instead of the usual discontinuities that appear in the first derivative in the Schrödinger scenario.

This puzzling situation has been discussed previously in the literature by many authors. Rigorous construction of self-adjoint extensions for the Dirac operator, allowing the handling of matching conditions at the support of the δ-potential, were discussed in [1]. Using their results, a discussion of this problem was presented in [2]. However, we have realized that the proposed solution corresponds to a different self-adjoint extension, associated also with a different singular potential.

At present, a simple and elementary discussion, without the necessity of invoking sophisticated mathematical constructions, is still not available in the literature. In this paper we want to overcome this situation, showing in elementary terms how to handle the problem in configuration space. Other authors have shown how to handle the problem in momentum space [3]. Using our results, we discuss the occurrence of supercritical effects, i.e. the possibility that the ground state starts to dive into the depths of the Dirac sea, implying positron emission [4].

The Dirac equation with an external potential can be written as

$$H\psi = E\psi \tag{1}$$

where

$$H = c\hat{\alpha} \cdot \hat{p} + \hat{\beta}mc^2 + V(r) \tag{2}$$

where $\hat{p} = -\mathrm{i}\hbar\nabla$. Here $\hat{\alpha}$ and $\hat{\beta}$ are the usual 4×4 Dirac matrices and ψ is the four-component Dirac spinor.

In what follows we will focus on the attractive spherically symmetric (vector) potential given by

$$V(r) = -a\delta(r - r_0) \tag{3}$$

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with $a > 0$.

It is convenient to recall some general properties of the solution of the Dirac equation in a central potential. For more details the reader may consult the book by Greiner *et al* [5] and references therein. In this case, the complete set of commuting operators is given by H, J^2, J_3 and K, where $\vec{J}$ is the total angular momentum (i.e. $\vec{J} = \vec{L} + \vec{S}$), and $\vec{K}$ is defined by

$$K = \beta(\vec{\Sigma} \cdot \vec{L} + \hbar \mathbb{I}). \tag{4}$$

In this expression $\vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}$ where the σ are the Pauli matrices. In terms of $\vec{\Sigma}$, $\vec{S} = \frac{\hbar}{2}\vec{\Sigma}$. On the other hand $\vec{L}$ is the orbital angular momentum. The eigenvalues of the operator K are given by

$$K\psi = -\kappa\hbar\psi = \pm(j + \tfrac{1}{2})\hbar\psi \tag{5}$$

where $\psi = \begin{pmatrix} \psi_u \\ \psi_l \end{pmatrix}$ is the four-component spinor solution of the Dirac equation written in terms of the two-component upper and lower ψ_{u} and ψ_{l}. In the equation (5), $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$ are the usual eigenvalues of J^2 according to

$$J^2\psi = j(j+1)\hbar^2\psi. \tag{6}$$

We note that the four-component Dirac spinor is not an eigenfunction of L^2. However, the upper and lower components, taken separately, satisfy

$$L^2\psi_{\mathrm{u}}(x) = [j(j+1)\hbar^2 + \kappa\hbar^2 + \tfrac{1}{4}\hbar^2]\psi_{\mathrm{u}}(x) \equiv l_u(l_u+1)\hbar^2\psi_{\mathrm{u}}(x) \tag{7a}$$

and

$$L^2\psi_{\mathrm{l}}(x) = [j(j+1)\hbar^2 - \kappa\hbar^2 + \tfrac{1}{4}\hbar^2]\psi_{\mathrm{l}}(x) \equiv l_l(l_l+1)\hbar^2\psi_{\mathrm{l}}(x). \tag{7b}$$

Note that the orbital parities of the upper and lower components have opposite signs. It is convenient to parametrize the four-component spinor by separating the radial and angular dependence according to

$$\Psi = \begin{bmatrix} \psi_u \\ \psi_l \end{bmatrix} = \begin{bmatrix} g(r)\Omega_{jl_u m}(\theta,\phi) \\ \mathrm{i}f(r)\Omega_{jl_l m}(\theta,\phi) \end{bmatrix} \tag{8}$$

where

$$\Omega_{jlm}(\theta,\phi) = \sum_{m',m_s} \left(lsj|m'm_s m\right) Y_{lm'}(\theta,\phi)\chi_{\frac{1}{2}m_s} \tag{9}$$

are the spherical spinors that carry out the angular part. Here we have coupled, through appropriate Clebsh–Gordan coefficients, the scalar spherical harmonics $Y_{lm'}(\theta,\phi)$ with the eigenfunctions of the spin given by the two-component spinors $\chi_{\frac{1}{2}m_s}$.

For this discussion we do not need the explicit form of the angular part. If we now consider the Dirac equation for a spinor parametrized in this way, it is not difficult to show that the radial components satisfy the following set of coupled differential equations:

$$\hbar c\left(\frac{\mathrm{d}F}{\mathrm{d}r} - \kappa\frac{F}{r}\right) = -(E - V(r) - mc^2)G(r) \tag{10a}$$

and

$$\hbar c\left(\frac{\mathrm{d}G}{\mathrm{d}r} + \kappa\frac{G}{r}\right) = (E - V(r) + mc^2)F(r) \tag{10b}$$

where $G(r) \equiv rg(r)$ and $F(r) \equiv rf(r)$. Because of the linear discontinuity of the spinor function, given by the delta potential, we need to fix the boundary conditions in the neighbourhood of the shell $r = r_0$. If we multiply equation (10*a*) by F, (10*b*) by G and then sum both expressions to remove the singular delta function, we obtain

$$F'F + G'G = \frac{2mcFG}{\hbar} + \kappa\frac{(F^2 - G^2)}{r\hbar c}. \tag{11}$$

In the previous expression, the primes denote radial derivatives. By integrating between $r_0 - \varepsilon$ and $r_0 + \varepsilon$ and taking then the limit when $\varepsilon \to 0$ we obtain

$$\lim_{\varepsilon\to 0}\int_{r_0-\varepsilon}^{r_0+\varepsilon}(F'F + G'G)\,\mathrm{d}r = \lim_{\varepsilon\to 0}\int_{r_0-\varepsilon}^{r_0+\varepsilon}\left(\frac{2mcFG}{\hbar} + \kappa\frac{\left(F^2 - G^2\right)}{r\hbar c}\right)\mathrm{d}r. \tag{12}$$

Assuming that the discontinuities of these functions are well behaved we find that

$$\lim_{\varepsilon\to 0}(F^2 + G^2)|_{r_0-\varepsilon}^{r_0+\varepsilon} = 0. \tag{13}$$

We may consider F and G as the real and imaginary parts of a function in $\mathbb{C}$. In this context, equation (13) expresses the fact that the absolute value of this function is constant when crossing the support of the δ-potential. This is in agreement with the condition established by Dittrich *et al* (see equation (3.5*a*) in [1]; see also the remarks after equation (21) in [2]). In fact, the absolute value of this function is continuous for all r.

If we set $F_{+,-} \equiv F(r_0 \pm \varepsilon)$ and $G_{+,-} \equiv G(r_0 \pm \varepsilon)$, (13) becomes

$$F_+^2 + G_+^2 = F_-^2 + G_-^2. \tag{14}$$

Now, as a second step, we multiply the differential equations by G and F, respectively, and subtract them to obtain

$$F'G - FG' = -\frac{(E - mc^2)}{\hbar c}G^2 + \frac{(E + mc^2)}{\hbar c}F^2 + 2\frac{\kappa GF}{\hbar cr} - \frac{a}{\hbar c}\delta(r - r_0)(F^2 + G^2). \tag{15}$$

Dividing by $F^2 + G^2$, which is continuous for all values of r, we can integrate in the neighbourhood of the shell radius

$$\lim_{\varepsilon\to 0}\int_{r_0-\varepsilon}^{r_0+\varepsilon}\frac{F'G - FG'}{(F^2 + G^2)}\,\mathrm{d}r = -\frac{a}{\hbar c}\lim_{\varepsilon\to 0}\int_{r_0-\varepsilon}^{r_0+\varepsilon}\delta(r - r_0)\,\mathrm{d}r. \tag{16}$$

By using

$$\frac{F'G - FG'}{(F^2 + G^2)} = \frac{1}{(F/G)^2 + 1}\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{F}{G}\right) \tag{17}$$

and since $\int \frac{1}{1+h^2(x)}\,\mathrm{d}[h(x)] = \arctan(h(x))$ we have

$$\lim_{\varepsilon\to 0}\left(\arctan\frac{F(r)}{G(r)}\right)\Bigg|_{r_0-\varepsilon}^{r_0+\varepsilon} = -\frac{a}{\hbar c}. \tag{18}$$

In this way, our second boundary condition can be written as

$$\arctan\frac{F_+}{G_+} - \arctan\frac{F_-}{G_-} = -\frac{a}{\hbar c}. \tag{19}$$

Expressing the coupling constant in units of $\hbar c$, we define the dimensionless parameter $\alpha \equiv \tan(a/\hbar c)$. Our second boundary condition can then be expressed as

$$\frac{F_+}{G_+} = \frac{(F_-/G_-) - \alpha}{1 + \alpha(F_-/G_-)}. \tag{20}$$

Except for an arbitrary phase, the last expression can be written as a matricial relation between the radial functions on both sides of the potential,

$$\begin{bmatrix} F_+ \\ G_+ \end{bmatrix} = \begin{bmatrix} \cos(a/\hbar c) & -\sin(a/\hbar c) \\ \sin(a/\hbar c) & \cos(a/\hbar c) \end{bmatrix}\begin{bmatrix} F_- \\ G_- \end{bmatrix} \equiv A\begin{bmatrix} F_- \\ G_- \end{bmatrix}. \tag{21}$$

This matrix A is unitary (actually orthogonal), $\det A = 1$, and contains the information for finding the eigenvalue equation for the bound states. Returning to our complex valued function with real and imaginary parts given by F and G, respectively, it is interesting to remark that δ manifests itself through a change of phase of this function, given by $\tan(a/\hbar c)$.

For the solutions of equations (10a) and (10b) corresponding to the free case, we may separate the space into two regions:
Region I, $r < r_0$,

$$G_{\mathrm{I}}(r) = A_I r \left(\frac{\pi}{2kr}\right)^{1/2} I_{l_\kappa+1/2}(kr) \tag{22}$$

$$F_{\mathrm{I}}(r) = A_I \frac{k\hbar c}{E+mc^2} r \left(\frac{\pi}{2kr}\right)^{1/2} I_{l_{-\kappa}+1/2}(kr). \tag{23}$$

Region II, $r > r_0$,

$$G_{\mathrm{II}}(r) = A_{II} r \left(\frac{\pi}{2kr}\right)^{1/2} K_{l_\kappa+1/2}(kr) \tag{24}$$

$$F_{\mathrm{II}}(r) = -A_{II} \frac{k\hbar c}{E+mc^2} r \left(\frac{\pi}{2kr}\right)^{1/2} K_{l_{-\kappa}+1/2}(kr). \tag{25}$$

The relations we are looking for reduce to

$$\frac{F_{\mathrm{I}}}{G_{\mathrm{I}}} = \frac{k\hbar c}{E+mc^2} \frac{I_{l_{-\kappa}+1/2}(kr)}{I_{l_\kappa+1/2}(kr)} \tag{26}$$

$$\frac{F_{\mathrm{II}}}{G_{\mathrm{II}}} = -\frac{k\hbar c}{E+mc^2} \frac{K_{l_{-\kappa}+1/2}(kr)}{K_{l_\kappa+1/2}(kr)}. \tag{27}$$

Taking into account that for the ground state, for $j = l + s = \frac{1}{2}$, we have $l_\kappa = 0$ and $l_{-\kappa} = 1$, we can write

$$I_{1/2}(kr) = \sqrt{\frac{2}{\pi kr}} \sinh(kr) \tag{28}$$

$$I_{3/2}(kr) = \sqrt{\frac{2}{\pi kr}} \left(\cosh(kr) - \frac{\sinh(kr)}{kr}\right) \tag{29}$$

$$K_{1/2}(kr) = \sqrt{\frac{\pi}{2kr}} \mathrm{e}^{-kr} \tag{30}$$

$$K_{3/2}(kr) = \sqrt{\frac{\pi}{2kr}} \mathrm{e}^{-kr} \left(1 + \frac{1}{kr}\right). \tag{31}$$

In these equations k denotes a wavenumber, $\hbar ck = \sqrt{m^2c^4 - E^2}$. In order to find the eigenvalues of the Hamiltonian, we evaluate (26) and (27) of r_0 and use the boundary condition (20). In this way we are led to solve the following transcendental equation:

$$\begin{aligned} \frac{k\hbar c}{E+mc^2}\left(1+\frac{1}{kr_0}\right) + \alpha\left(\frac{k\hbar c}{E+mc^2}\right)^2\left(1+\frac{1}{kr_0}\right)\left(\frac{1-\tanh(kr_0)}{\tanh(kr_0)}\right) \\ = \frac{k\hbar c}{E+mc^2}\left(\frac{1-\tanh(kr_0)}{\tanh(kr_0)}\right) - \alpha. \end{aligned} \tag{32}$$

Without solving explicitly this equation, we can analyse the behaviour of the ground state energy E, as a function of the parameter $\alpha = \tan(a/\hbar c)$, related to the coupling constant a. We start by introducing the following dimensionless variables:

$$\varepsilon \equiv \frac{E}{mc^2} \tag{33a}$$

$$\rho \equiv \frac{r_0}{\hbar/mc} \tag{33b}$$

$$s_0 \equiv \rho\sqrt{1-\varepsilon^2} \tag{33c}$$

$$u_0 \equiv \rho(1+\varepsilon) \tag{33d}$$

$$g_0 \equiv \frac{\tanh(kr_0)}{kr_0}. \tag{33e}$$

In terms of these variables, our eigenvalue equation (32) can be written as

$$\alpha = \frac{s_0u_0(1+g_0s_0)}{u_0{}^2-(s_0+1)s_0(1-g_0)}. \tag{34}$$

For a fixed value of the radius of the δ-shell, r_0 (with $r_0 \neq 0$), we are interested in determining the existence of the ground state energy in the interval $(-mc^2, mc^2)$ (i.e. $-1 \leqslant \varepsilon \leqslant 1$). The existence of an ε in this range will depend on the values of the coupling constant a through the dimensionless parameter α.

Since $\hbar ck = \sqrt{m^2c^4 - E^2} = mc^2\sqrt{1-\varepsilon^2}$, we obtain from (33*e*) that

$$\lim_{\varepsilon\to\pm 1} g_0 = 1. \tag{35}$$

On the other hand, using (33*e*) we obtain

$$\lim_{\varepsilon\to -1} \frac{1-g_0}{u_0} = \frac{2}{3}\rho. \tag{36}$$

Using the limits (35) and (36) in equation (34) we see that as E approaches the free state (i.e. $\varepsilon \to 1^-$), $\alpha \to 0^+$, which agrees with the fact that the bound states disappears for a vanishing potential.

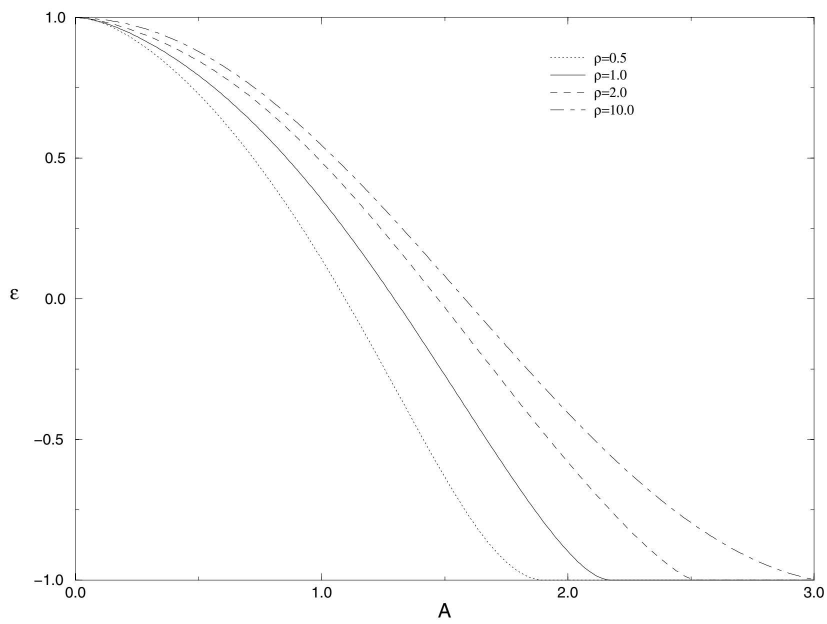

Figure 1. In figure 1, we show the behaviour of the ground state energy $\varepsilon = E/mc^2$, for different values of the size $\rho = r_0/(\frac{\hbar}{mc})$ of the delta-shell as a function of the dimensionless coupling constant $A = a/(\hbar c)$: $\rho = 0.5$ (dotted curve), $\rho = 1.0$ (solid curve), $\rho = 2.0$ (dashed curve), $\rho = 10.0$ (dot–dashed curve).

Proceeding as before, with $\varepsilon \to -1^+$ (i.e. as the energy approaches the Dirac sea), we infer from equation (34) that α approaches the value $-3/2\rho$, which gives

$$\tan\left(\frac{a_{\rm crit}}{\hbar c}\right) = -\frac{3}{2\rho} \tag{37}$$

where $a_{\rm crit}$, the minimum positive solution of (37), is the value of the coupling constant for which the ground state energy sinks into the Dirac sea (e.g. for $\rho = 1$, $a_{\rm crit} = 2.19\hbar c$).

The numerical solution of equation (34) for the dimensionless ground state energy ε as a function of ρ and a is plotted in figure 1. Notice that for a fixed value of ρ, ε is a decreasing function of a. For all finite values of ρ there are supercritical effects. Clearly, the value of $a_{\rm crit}$ for which ε sinks into the Dirac sea increases with ρ. However, the limit $r_0 \to 0$ is not well defined in (34) and thus we cannot find solutions for bound states in this limit. We would like to remark that a general theorem by Svendsen [6, 7], tells us that supercritical effects are absent in this limit.

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