Comment on "Zero-range potentials for Dirac particles: Scattering and related continuum problems"

F. A. B. Coutinho[1] and Y. Nogami[2]
[1]*Faculdade de Medicina, Universidade de São Paulo, 01246-903, SP, Brazil*
[2]*Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada L8S 4M1*

(Received 4 August 2005; published 10 February 2006)

In a recent paper, Szmytkowski proposed zero-range potentials for Dirac particles in three space dimensions. On the other hand, there is a theorem, proved by Svendsen a long time ago, which implies that zero-range potentials cannot be defined for the Dirac equation in two and three space dimensions. We discuss a difficulty that underlies Szmytkowski's approach.

DOI: 10.1103/PhysRevA.73.026701 PACS number(s): 03.65.Nk

In a recent paper, Szmytkowski proposed zero-range potentials (ZRPs) for Dirac particles in three space dimensions [1]. On the other hand, there is a theorem, proved by Svendsen a long time ago, which implies that ZRPs cannot be defined for the Dirac equation in two and three space dimensions [2,3]. We discuss a difficulty that underlies Szmytkowski's approach.

Let us focus on the three-dimensional case with only one ZRP at the origin. Before examining the relativistic case, let us briefly review the nonrelativistic case. With the Schrödinger equation there is no difficulty in defining the ZRP; it can be done as follows. Consider a particle of mass m bound by a central attractive square-well potential with range a and depth D. (Actually the potential can be repulsive as we point out later.) Following the standard procedure, we match the Schrödinger wave function for a stationary S state and its derivative $\psi(r)$ and $d\psi(r)/dr$ at $r=a$ and obtain

$$\kappa_0 a \cot(\kappa_0 a) = \kappa a, \tag{1}$$

where $\kappa=(-2mE)^{1/2}, \kappa_0=[2m(E+D)]^{1/2}$ and E is the energy of the bound state. We are using units such that $c=\hbar=1$. For given values of D and a, Eq. (1) can be solved for E (or for κ). Assume that there is a bound state with $E<0$.

Consider the zero-range limit in which $a\to 0$ and $D\to\infty$. If we take this limit such that $Da^3 \equiv g$ is kept constant, then $E\to-\infty$, i.e., the bound state collapses [4]. This can be avoided by scaling D in such a way that the value of κ remains fixed [3]. The value of κ, and hence the energy E, can be chosen at will. The ZRP that we obtain in this way is characterized by κ (or E) rather than by $g=Da^3$ which vanishes in this limit.

The ZRP introduced above is equivalent to the ZRP represented by the boundary condition

$$\lim_{r\to 0}\left(\frac{d}{dr}+\kappa\right)r\psi(r)=0. \tag{2}$$

This requires that $\psi(r)$ behave as $e^{-\kappa r}/r$ in the vicinity of the origin. [This is in contrast to the usual assumption that $r\psi(r)\to 0$ as $r\to 0$, which follows from Eq. (2) with $\kappa\to\infty$.] Wave function $\psi(r)$ is normalizable. Boundary condition (2) can be rewritten in the form of Eq. (2.5) (with $\mathbf{r}_n=0$) of Szmytkowski and Gruchowski [5], which they used in defining a ZRP for the Schrödinger equation. Let us add that, unlike the $\kappa(E)$ of Ref. [5], our κ is independent of E but this difference is unimportant in the context of the present note.

We assumed above that there is a bound state but this assumption is not essential. If there is no bound state, depth D and range a can be scaled such that a given scattering length be obtained. In this way we can also handle a repulsive potential (with negative D). Thus we obtain a one-parameter family of ZRPs for the Schrödinger equation. This is well known. See the literature quoted in Ref. [3].

Let us now turn to the relativistic case with the Dirac equation. One would naturally try to define a ZRP for the Dirac equation in a manner similar to what we described above. Starting with a square-well potential of a finite range and taking an appropriate limit, one can define a ZRP that gives a bound state solution with a specified energy eigenvalue or a scattering length. As was shown explicitly in Ref. [3], however, the solutions of the Dirac equation with the so-constructed ZRP is not acceptable. This is because the lower component of the Dirac wave function (with a positive energy) is so singular that the wave function is not normalizable. As we emphasized in Ref. [3], to find a wave function that satisfies the Dirac equation together with a given boundary condition is one thing but whether the solution is physically acceptable is another. The unnormalizability of the associated wave function leads us to realize that ZRPs are impossible for the Dirac equation in three dimensions. An exactly similar situation is found in the two dimensional case. This is how a consequence of Svendsen's highly mathematical theorem can be interpreted [2,3].

Szmytkowski [1] defined ZRPs for the Dirac equation by means of his boundary condition (2.18), which is a relativistic extension of Eq. (2.5) of Ref. [5] and is equivalent to specifying the scattering length. Consider the scattering problem with a ZRP at the origin with $\mathbf{r}_1=0$. Szmytkowski's wave function is of the form of

$$\Psi^{(+)}(E,\mathbf{r}) = \Phi(E,\mathbf{r}) + \Psi_1^{(+)}(E,\mathbf{r}), \tag{3}$$

where $\Phi(E,\mathbf{r})$ represents the incident wave and $\Psi_1^{(+)}(E,\mathbf{r})$ the scattered wave. The latter is given by

$$\Psi_1^{(+)}(E,\mathbf{r}) = \begin{pmatrix} h_0(kr)\chi(E) \\ \epsilon h_1(kr)(\hat{\mathbf{r}}\cdot\sigma)\chi(E) \end{pmatrix}, \tag{4}$$

$$h_0(z) = \frac{e^{iz}}{z}, \quad h_1(z) = \frac{e^{iz}}{z} + \frac{ie^{iz}}{z^2}. \tag{5}$$

Here $\hat{\mathbf{r}} = \mathbf{r}/r$, k and ϵ are constants related to E and $\chi(E)$ is a two-component spinor. For details, see Ref. [1]. The $\Psi_1^{(+)}(E,\mathbf{r})$ is a free wave function, which can be made to satisfy the boundary condition at the origin by appropriately choosing $\chi(E)$. Note that the lower component of $\Psi_1^{(+)} \times (E,\mathbf{r})$ behaves as e^{ikr}/r^2 near the origin. This singular behavior makes $\Psi^{(+)}(E,\mathbf{r})$ not square integrable. It is a standard practice to normalize the wave function such that

$$\int \Psi^{(+)\dagger}(E',\mathbf{r})\Psi^{(+)}(E,\mathbf{r})d\mathbf{r} = \lambda\,\delta(k'-k),$$

where λ is a finite constant. This cannot be done for the above wave function.

Szmytkowski considered only scattering states but his analysis can be extended to include bound states. One can set up a ZRP by means of a boundary condition which specifies the binding energy. Alternatively, as was done in Ref. [3], one can start with a square-well potential that supports a bound state and take its zero-range limit in such a way that the binding energy remains fixed. The wave function of the bound state that ensues is given by Eq. (3.18) of Ref. [3], which is exactly in the same form as the $\Psi_1^{(+)}(E,\mathbf{r})$ quoted above but with k replaced by $i\kappa$. (There is no incident wave in the bound state.) Its lower component contains a derivative of the upper component and diverges as $e^{-\kappa r}/r^2$ around the origin. The wave function is not normalizable and hence the underlying ZRP is physically unacceptable.

Even if $\Psi_1^{(+)}(E,\mathbf{r})$ is not normalizable one can mathematically proceed to examine the scattering phase shifts and scattering cross section as was done in Ref. [1]. These quantities are related to the wave function at large distances. For problems such that the wave function near the origin is irrelevant, the formulas developed in Ref. [1] could be used. However, if one evaluates a matrix element of some physical quantity by using such unnormalizable wave functions, one may obtain a misleading result.

We have focused on the three-dimensional case. The situation of the two-dimensional case is similar. As was explicitly shown in Ref. [3], the lower component of the Dirac wave function in two dimensions with a ZRP behaves like $1/r$ and hence is not square integrable in two dimensions [6].

The Schrödinger equation can usually be regarded as a nonrelativistic limit of the Dirac equation. In this sense it may appear strange that ZRPs are possible for the Schrödinger equation but not for the Dirac equation. This disparity stems from the following. In deriving the Schrödinger equation from the Dirac equation, we let the ratio of the potential $V(r)$ over mass m tend to zero. Then the lower component of the Dirac wave function disappears (even if it is singular) while the upper component is reduced to the Schrödinger wave function. In defining the ZRP for the Dirac equation as we explained above, this ratio becomes infinite. Recall that we let $D/m \to \infty$ no matter how large m is. This is how the difference between the situations with the Dirac and Schrödinger equations arises. A difference of a similar nature arises regarding the ZRPs for the Schrödinger equation and the Dirac equation in one space dimension, although in this case ZRPs are possible for the Dirac equation also [7].

This work was supported by the Fundação de Amparo à Pesquisa do Estado de São Paulo, Conselho Nacional de Desenvolvimento Científico e Tecnológico and the Natural Sciences and Engineering Research Council of Canada.

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