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Zero-range potential for the Dirac equation in two and three space dimensions: Elementary proof of Svendsen's theorem

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There is a theorem proved by Svendsen which implies that a zero-range (δ -function) potential cannot be defined for the Dirac equation in two and three space dimensions. We give an elementary proof of the theorem by examining the solution of the Dirac equation with a square-well potential of finite range and taking the zero-range limit.

I. INTRODUCTION

In nonrelativistic quantum mechanics, the zero range or the δ -function potential in one space dimension, say $-g\delta(x)$, is well defined with no ambiguity. For its simplicity the one-dimensional δ -function potential is used extensively as a model interaction in condensed-matter physics and also as classroom exercises of quantum mechanics. The δ -function potential can also be used with the relativistic Dirac equation in one dimension. Unlike the nonrelativistic case, there is an arbitrariness regarding the definition of the δ function in the relativistic case.¹⁻³ However, there is nothing really serious about this arbitrariness.

In two and three dimensions, the δ -function potential could be defined by starting with a square-well potential of depth D and radius a , and taking the limit of $a \rightarrow 0$, but keeping $Da^n \equiv g$ constant, where n ($=2$ or 3) is the dimensionality of the space. The g is essentially the strength of the δ -function potential. We are interested in an attractive potential such that there is at least one bound state. In nonrelativistic quantum mechanics with the Schrödinger equation, it is well known that the ground-state energy becomes $-\infty$ in the δ -function limit of $a \rightarrow 0$. However, the strength g of the potential can be scaled or renormalized such that there is a ground state with a finite binding energy. In this sense one can define the δ -function potential for the Schrödinger equation in two and three dimensions.⁴ In Sec. II we will briefly summarize how the δ -function potential can be defined for the Schrödinger equation in two and three dimensions.

We are naturally interested in the relativistic extension

of the notion of the δ -function potential in two and three dimensions. Unfortunately, this is not possible, according to Svendsen, who proved a theorem that has important implications regarding the possibility of the δ -function potential.⁵ As an application of the theorem, Svendsen examined the kinetic-energy operator of the Dirac Hamiltonian defined within a set of functions that vanish near the origin. He found that the operator so defined is essentially self-adjoint if the dimensionality of space is greater than 1, which excludes the possibility of the δ -function potential for the Dirac equation for other than one dimension. Since Svendsen's paper is highly mathematical, it would be interesting to examine the problem in a more elementary way by starting with a square-well potential and taking the zero-range limit. This we will do in Sec. III.

Although the δ -function potential for the Dirac equation in two and three dimensions cannot be defined, there is no such problem with the δ -shell potential, provided that the radius of the shell is not zero. We will discuss this in the Appendix. We use natural units ($c = \hbar = 1$) throughout.

II. SCHRÖDINGER EQUATION IN TWO AND THREE DIMENSIONS

We confine ourselves to the S state. The Schrödinger equation reads

$$-\frac{1}{2m} \left[\frac{d^2\psi}{dr^2} + \frac{n-1}{r} \frac{d\psi}{dr} \right] + V\psi = E\psi, \quad (2.1)$$

where n ($=2$ or 3) is the dimensionality. For the potential $V(r)$ we assume an attractive square well;

$$V(r) = \begin{cases} -D & \text{for } r < a \\ 0 & \text{for } r > a \end{cases} \quad (2.2)$$

Following the standard method, ψ and $d\psi/dr$ for $r > a$ and $r < a$ are matched at $r = a$, which leads to the following equations:

$$\kappa_0 a J_1(\kappa_0 a) / J_0(\kappa_0 a) = \kappa a K_1(\kappa a) / K_0(\kappa a) \quad \text{for } n = 2 \quad (2.3)$$

and

$$\kappa_0 a \cot(\kappa_0 a) = \kappa a \quad \text{for } n = 3, \quad (2.4)$$

where $\kappa = (-2mE)^{1/2}$, $\kappa_0 = [2m(D + E)]^{1/2}$, and the J 's and K 's are Bessel and modified Bessel functions, respectively. For given values of D and a , Eqs. (2.3) and (2.4) determine E for $n = 2$ and 3 , respectively.

Let us consider the limit such that $D \rightarrow \infty$, $a \rightarrow 0$, but $Da^n = g = \text{const}$ and $|E|$ is finite. Then $\kappa_0 \simeq (2mD)^{1/2}$, and

$$\kappa_0 a \rightarrow \begin{cases} (2mg)^{1/2} < \infty & \text{for } n = 2 \\ (2mg/a)^{1/2} \rightarrow \infty & \text{for } n = 3 \end{cases} \quad (2.5)$$

It is not difficult to see that, as long as E remains finite, Eqs. (2.3) and (2.4) cannot be satisfied in this limit. For $n = 2$, for example, the left-hand side of Eq. (2.3) approaches a constant, whereas the right-hand side diverges; recall that, for $x \ll 1$, $K_0(x) \simeq -[\ln(x/2) + \gamma]$, where $\gamma = 0.577\dots$ is the Euler constant, and $K_1(x) \simeq 1/x$.

This difficulty can be avoided by scaling D in such a way that

$$\kappa_0 a \simeq \begin{cases} \{-2/[\ln(\kappa a/2) + \gamma]\}^{1/2} & \text{for } n = 2 \\ (\pi/2) + 2\kappa a/\pi & \text{for } n = 3 \end{cases} \quad (2.6)$$

The value of κ , and hence the energy E , can be chosen at will. The δ -function potential is accordingly determined, albeit $g = Da^n \rightarrow 0$. The parameter of this potential is therefore the bound-state energy or κ rather than g . Let us add that the renormalization trick summarized above does not work for dimensions higher than 3; this also follows from Svendsen's theorem.⁵ When the angular part is separated and the Schrödinger equation is written for $r\psi$, the kinetic energy in n dimensions bears the "dimensional barrier" $[(n-1)(n-3)/4]/(2mr^2)$.^{6,7} This makes the δ -function potential impossible for dimensions greater than 3.

III. DIRAC EQUATION IN TWO AND THREE DIMENSIONS

The Dirac equation reads

$$\{\boldsymbol{\alpha} \cdot \mathbf{p} + \beta[m + S(r)] + V(r)\}\psi = E\psi, \quad (3.1)$$

where $S(r)$ and $V(r)$ are a Lorentz scalar and (the zeroth component of) a vector. For each of S and V , we assume a square-well potential of the form of Eq. (2.2). Following, e.g., Schiff,⁸ we can separate the angular variables and reduce Eq. (3.1) to

$$[\boldsymbol{\alpha}_r \cdot \mathbf{p}_r + i\boldsymbol{\alpha}_r \cdot \boldsymbol{\beta} k/r + \beta(m + S) + V]\psi = E\psi, \quad (3.2)$$

where $\boldsymbol{\alpha}_r = \boldsymbol{\alpha} \cdot \mathbf{r}/r$ and $\mathbf{p}_r = -i[\partial/\partial r + (n-1)/(2r)]$, and

$$k = \begin{cases} L + (\beta/2) & \text{for } n = 2 \\ \beta(\boldsymbol{\sigma} \cdot \mathbf{L} + 1) & \text{for } n = 3 \end{cases}, \quad (3.3)$$

where $\boldsymbol{\sigma}$ is the Pauli spin matrix. For $n = 2$, $L \equiv xp_y - yp_x$. Since k commutes with H , we can take it as a constant. For the state that corresponds to the ground S state of the Schrödinger case, $k = \frac{1}{2}$ for $n = 2$, and $k = 1$ for $n = 3$. In the following we consider only these states. For the matrices $\boldsymbol{\alpha}_r$ and $\boldsymbol{\beta}$, we use $\boldsymbol{\alpha}_r = \boldsymbol{\sigma}_y$ and $\boldsymbol{\beta} = \boldsymbol{\sigma}_z$. If we denote the upper and lower components of ψ by u and v , respectively, Eq. (3.2) becomes

$$(m + S - E + V)u - \left[\frac{d}{dr} + \frac{n-1}{r} \right] v = 0, \quad (3.4)$$

$$\frac{du}{dr} + (-m - S - E + V)v = 0. \quad (3.5)$$

Let us first consider the two-dimensional case. For $r > a$, u and v are given by

$$u = K_0(\kappa r), \quad (3.6)$$

$$v = -\kappa K_1(\kappa r)/(m + E), \quad (3.7)$$

where $\kappa = (m^2 - E^2)^{1/2}$. For $r < a$ there are two cases:

$$(E - V)^2 - (m + S)^2 = \kappa_0^2 > 0 \quad (\text{case I}), \quad (3.8)$$

$$(m + S)^2 - (E - V)^2 = \kappa_0^2 > 0 \quad (\text{case II}). \quad (3.9)$$

Let us examine case I in some detail. Apart from the normalization factor, the solution for $r < a$ is given by

$$u = J_0(\kappa_0 r), \quad (3.10)$$

$$v = -\kappa_0 J_1(\kappa_0 r)/(m + E + E - V). \quad (3.11)$$

The continuity of u and v at $r = a$ leads to

$$\frac{\kappa_0}{m + S + E - V} \frac{J_1(\kappa_0 a)}{J_0(\kappa_0 a)} = \frac{\kappa}{m + E} \frac{K_1(\kappa a)}{K_0(\kappa a)}. \quad (3.12)$$

Suppose that $S = 0$ and $V = -D \rightarrow -\infty$; then $\kappa_0 \simeq D$. We now take the limit of $a \rightarrow 0$. It appears as if we can define the δ -function potential by scaling the well depth D such that

$$\kappa_0 a \simeq x_0 + \xi(a), \quad (3.13)$$

where x_0 is such that $J_0(x_0) = 0$, and $\xi(a)$ is a function of a such that $\xi \rightarrow 0$ as $a \rightarrow 0$. When $\xi \ll 1$, $J_0(\kappa_0 a) \simeq -\xi$, and the left-hand side of Eq. (3.12) becomes $\simeq -1/\xi$. Therefore, if we choose $\xi(a)$ to be

$$\xi(a) = a(m + E)[\ln(\kappa a/2) + \gamma], \quad (3.14)$$

the Dirac equation is satisfied with the eigenvalue E , which is specified by κ . This remains valid in the limit of $a \rightarrow 0$.

To find a solution of the Dirac equation is one thing, but whether or not the solution is physically acceptable is another. Unfortunately, ψ obtained above by scaling κ_0

becomes unnormalizable in the limit of $a \rightarrow 0$. This is due to the behavior of v near the origin; $v \simeq -1/r$ and hence $\int v^2 r dr$ diverges.

In the case II of Eq. (3.9), we can assume that S dominates. In this case it turns out that it is impossible to scale the depth of the potential in such a way that the Dirac equation remains satisfied in the limit of $a \rightarrow 0$. But even if the scaling were possible, v would acquire essentially the same singularity at the origin as in case I. Hence the δ -function potential cannot be defined.

The three-dimensional case is very similar. The three-dimensional counterpart of Eq. (3.12) is⁹

$$\frac{\kappa_0 a \coth(\kappa_0 a) - 1}{m + S + E - V} = -\frac{\kappa a + 1}{m + E}. \quad (3.15)$$

In taking the limit of $a \rightarrow 0$, the scaling can be done such that

$$\kappa_0 a \rightarrow \pi + (m + E)a. \quad (3.16)$$

The Dirac equation is satisfied with the eigenvalue E . However, the difficulty regarding the normalizability of the wave function again develops. Apart from a constant factor, the two components of ψ for $r > a$ in three dimensions are given by

$$u = e^{-\kappa r} / (\kappa r), \quad (3.17)$$

$$v = -e^{-\kappa r} (1 + \kappa r) / [(m + E)\kappa r^2]. \quad (3.18)$$

In the limit of $a \rightarrow 0$, v becomes unnormalizable.

IV. DISCUSSION

We have examined the solutions of the Dirac equation of a square-well potential in two and three space dimensions and examined the zero-range limit with an eye to define the δ -function potential. We had a partial success in the sense that the solution of the Dirac equation with the vector potential can be retained in this limit. However, the wave function becomes unnormalizable and hence unacceptable. This negative result is in accord with Svendsen's theorem regarding the self-adjointness of the kinetic-energy operator for the Dirac particle.

In order to see the impossibility of the δ -function potential, actually it was unnecessary to examine the eigenvalue equation (3.12) or (3.15). Inspection of v near the origin suffices to see that the δ -function potential is not allowed, irrespective of whether or not the relevant eigenvalue equation has a solution. The reason why we examined the eigenvalue problem and then the scaling procedure is that we were curious about the nature of the operator consisting of the Dirac kinetic energy and the renormalized δ -function potential. This operator has continuous spectra for $|E| > m$ and one discrete energy between m and $-m$. However, it can be shown that the square-well potential in its δ -function limit has no effect on the continuum; the scattering phase shifts are all zero.¹⁰ Therefore, the scattering states, which are the same as those of the free Dirac equation, and the discrete state form an overcomplete set of functions. This implies that the operator under consideration is not self-adjoint.

Regarding the δ -function potential, the Dirac and Schrödinger equations are very different; in two and three dimensions, the δ -function potential can be defined for the latter, but not for the former. This may sound strange in view of the usual interpretation that the Schrödinger equation is an approximation to the Dirac equation. This difference stems from the following. In obtaining the δ function as the narrow-width limit of the square well, the depth of the well is made much greater than the mass in the relativistic case. On the other hand, in reducing the Dirac equation to the Schrödinger equation, it is understood that the mass is much greater than the strength of the potential; in this sense, the depth cannot exceed the mass.

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APPENDIX: δ -SHELL POTENTIAL

Let us consider the attractive δ -shell potential of the form

$$S(r) = -g_S \delta(r - a), \quad V(r) = -g_V \delta(r - a), \quad (A1)$$

where the g 's are both positive. The definition of this potential is beset with exactly the same type of ambiguity as that of the δ -function potential in one dimension.¹ For simplicity, let us adopt the definition by means of

$$\int \delta(r - a) f(r) dr = [f(a +) + f(a -)] / 2, \quad (A2)$$

where $f(r)$ stands for $u(r)$ or $v(r)$, and $a +$ means a plus a positive infinitesimal. It turns out that, in general, u and v are both discontinuous at $r = a$. There is an alternative definition of the potential, which is obtained by starting with a shell of a finite width and then taking the zero-width limit. The u and v which follow from this latter definition of the δ -shell potential do not satisfy Eq. (A2), but we do not discuss this aspect here.¹¹

We confine ourselves to the usual ground state that we have considered in the main text. Equations (3.4) and (3.5) lead to

$$-g(u_+ + u_-) / 2 = v_+ - v_-, \quad (A3)$$

$$g'(v_+ + v_-) / 2 = u_+ - u_-, \quad (A4)$$

where $u_+ \equiv u(a +)$, $u_- \equiv u(a -)$, etc., and

$$g = g_S + g_V, \quad g' = -g_S + g_V. \quad (A5)$$

Equations (A3)–(A5) can be reduced to a single equation:

$$(4 - gg')(u_+ v_- - u_- v_+) - 4(gu_+ u_- + g'v_+ v_-) = 0. \quad (A6)$$

The above boundary condition applies to both of two and three dimensions.

Apart from a common constant factor, u and v for

$r > a$ are given by Eqs. (3.5) and (3.6), respectively, in two dimensions, and by Eqs. (3.17) and (3.18) in three dimensions. For $r < a$, the K_0 and K_1 of two dimensions are replaced by I_0 and $-I_1$, respectively. Note that κ_0 of Eq. (3.8) or (3.9) does not appear because the potential is zero except at $r = a$. In three dimensions, u and v of $r < a$ are given by

$$u = \sinh(\kappa r) / (\kappa r), \quad (\text{A7})$$

$$v = [\cosh(\kappa r) - \sinh(\kappa r) / (\kappa r)] / (m + E)r. \quad (\text{A8})$$

Equation (A6) together with these wave functions leads to

$$4 - gg' = 4a [g(m + E)K_0 I_0 - g'(m - E)K_1 I_1] \quad (\text{A9})$$

for $n = 2$,

where $K_0 \equiv K_0(\kappa a)$, etc., and

$$4 - gg' = 4\kappa^{-1} e^{-x} \sinh x [g(m + E) - g'(m - E) \times (1 + x^{-1})(\coth x - x^{-1})] \quad (\text{A10})$$

for $n = 3$,

where $x = \kappa a$. These equations determine the eigenvalue of a bound state, if any. In the limit of $a \rightarrow 0$, the wave function becomes unnormalizable. The scattering phase shift can be calculated; it vanishes as $a \rightarrow 0$.

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⁴There is a long history of the interest in the δ -function interaction: See, e.g., L. H. Thomas, *Phys. Rev.* **47**, 903 (1935); G. Breit, *Phys. Rev.* **71**, 215 (1947); R. A. Minlos and L. D. Fadeev, *Zh. Eksp. Teor. Fiz.* **41**, 1850 (1961) [*Sov. Phys.—JETP* **14**, 1315 (1962)]; L. W. Bruch and J. A. Tjon, *Phys. Rev. A* **19**, 425 (1979); G. Flamand, in *Cargèse Lectures in Theoretical Physics*, edited by F. Lurcat (Gordon and Breach,

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⁹The Dirac equation with the square-well potential has been discussed in detail by W. Greiner, B. Müller, and J. Rafelski, *Quantum Electrodynamics of Strong Fields* (Springer-Verlag, Berlin, 1985), pp. 71–79. Our u and v correspond to their g and f , respectively.

¹⁰In the nonrelativistic case the renormalized δ -function potential gives rise to a nonvanishing S -wave phase shift. See Fernando Perez *et al.* and Lloyd of Ref. 4 for the two- and three-dimensional cases, respectively.

¹¹See, in particular, Calkin *et al.* quoted in Ref. 1.