Ambiguities with the relativistic δ-function potential

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By explicit calculation on the one-dimensional Dirac equation, we exhibit an ambiguity in defining the relativistic δ-function potential.

In many cases of physical interest, the δ-function potential is a very convenient approximation to more structured, and more difficult, short-ranged potentials. In relativistic theories, its use is often mandated because only a mathematical point has a relativistically invariant shape. Nevertheless, we were surprised recently to find difficulties and ambiguities regarding its use. Problems appear even in the case of *one-body* point scatterers, although it is generally assumed that all problems and paradoxes concerning one-body potentials have been resolved since the beginning of relativistic quantum theory. Nevertheless, the difficulties—and their resolution—that we point out in the present work have apparently not, as far as we are aware, been analyzed before.

Previously, we noted[1] some difficulties regarding the use of *two-body* forces in one spatial dimension. For arbitrary potentials, we discovered that Schrödinger's equation without mass possesses a "strange" set of eigenfunctions which, in most applications, one would rule inadmissible on physical grounds. The problems could be traced to the kinetic energy, which, being linear in the momenta, has no lower bound. Indeed, filling the Fermi-Dirac sea had the effect of restoring the lower bound and thus eliminating the strange solutions in favor of physically admissible states.

In the present study we observe that generally, with the inclusion of a mass, one-body potentials are less pathologic, but that, nevertheless, the limit of a δ function presents its own peculiar difficulties. Such difficulties, arising from very steep or deep potentials, have long been known to exist in relativistic equations. Klein's famous paradox (transmission coefficient exceeding unity) comes from potentials which "punch a hole" in the sea of negative energy states, as a δ function surely does. However, our findings seem to be unrelated to this classic paradox, although of course our considerations are based on similar equations.

What we have observed is that as potentials of different "shapes" approach the δ-function limit of zero width and constant area, the resulting eigenfunctions approach different values at the discontinuity. The resulting phase shifts, transmission coefficients, etc., are, therefore, all different. In particular, where cutoffs are used, the solutions will depend explicitly on the cutoffs and on the manner in which they are taken. This is a most unfortunate situation, which is only somewhat alleviated by the observation that all *reasonable* methods agree in weak coupling, i.e., to leading order in c/m, where c is the strength of the δ-function potential. (We have chosen units such that the speed of light is unity.)

We now examine solutions of the one-particle Dirac equation in one dimension with a mass term. In a basis of left- and right-going particles—or the no-mass basis—the Hamiltonian eigenvalue equation has the following form:

$$H\Psi = \left(-i\sigma_z \frac{d}{dx} + V - m\sigma_x\right)\Psi = \omega\Psi . \tag{1}$$

We emphasize that H is here given in configuration space. The potential V is a local potential which we will examine in detail. The 2×2 matrices are the Pauli spin matrices:

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$
$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2}$$

Outside the region of interaction, $V=0$, so we look for solutions of the form

$$\Psi = e^{ikx}\phi . \tag{3}$$

The spinor ϕ obeys the equation

$$(\omega I + m\sigma_x - k\sigma_z)\phi = 0 , \tag{4}$$

and thus

$$\det(\omega I + m\sigma_x - k\sigma_z) = 0 = \omega^2 - k^2 - m^2 . \tag{5}$$

A convenient parametrization of this dispersion relation is

$$\omega = m\cosh\theta , \quad k = m\sinh\theta , \tag{6}$$

and solutions correspond to

(a) $\mathrm{Im}\theta = 0$, positive energy states,

(b) $\mathrm{Im}\theta = \pi$, negative energy states,

(c) $\mathrm{Re}\theta = 0$, bound states.

Upon returning to Eq. (4), the spinor $\phi(\theta)$ is determined to be

$$\phi(\theta) = \frac{1}{(2\cosh\theta)^{1/2}} \begin{pmatrix} e^{\theta/2} \\ -e^{-\theta/2} \end{pmatrix}. \tag{7}$$

To simplify notation, we henceforth set the mass $m = 1$.

We now must determine the solution within the interaction region $|x| < \alpha/2$ in order to connect solutions on the left with solutions on the right. We want to consider local potentials, or potentials of the δ-function type—that is, potentials which vanish for $|x| > \alpha/2$, yet $V \neq 0$ for $|x| < \alpha/2$, and $\alpha \to 0$, $|V| \to \infty$. In fact, we wish to consider more general potentials than simply those diagonal in configuration space. Our two examples in this paper will be

(a) a configuration potential

$$V = \delta(x - x')g, \quad |x| < \alpha/2$$
$$\to c\delta(x - x')\delta(x), \tag{8a}$$

as $g \to \infty$, $\alpha \to 0$, and $c = g\alpha$;

(b) a separable potential

$$V = g, \quad |x| < \alpha/2, \quad |x'| < \alpha/2$$
$$\to c\delta(x)\delta(x') \tag{8b}$$

as $g \to \infty$, $\alpha \to 0$, and $c = g\alpha^2$.

Note that both potentials appear to approach the same limit as $\alpha \to 0$. However, much to our surprise, we have found that the solutions do not in fact approach the same limit. This is in contrast to the nonrelativistic case, as we shall verify.

Thus, to summarize, we consider potentials of the form

$$V = gv(x, x'), \quad |x| < \alpha/2 \tag{9}$$

where

$$\int_{-\alpha/2}^{\alpha/2} dx \int_{-\alpha/2}^{\alpha/2} dx' V = c, \tag{10}$$

as $\alpha \to 0$, $g \to \infty$, and c is constant.

Inside the interaction region $|x| < \alpha/2$, the potential is very large in magnitude since g is large in magnitude, and thus we can neglect both the mass and energy terms of the Dirac equation (1). We are thus left with two uncoupled equations for the two components of ψ_j, $j = 1, 2$ of ψ:

$$i(-1)^j \frac{d\psi_j}{dx} + g\int_{-\alpha/2}^{\alpha/2} dx' v(x, x')\psi_j(x') = 0. \tag{11}$$

Assume for the moment we have solved this linear integrodifferential equation for $\psi_j(x)$, $|x| < \alpha/2$. We may then require continuity of the spinors at $x = \pm\alpha/2$. Since we are interested in the limit $\alpha \to 0$, these become

$x = \alpha/2 \to 0+$:

$$a\phi(\theta) + b\phi(-\theta) = \begin{vmatrix} \psi_1(0+) \\ \psi_2(0+) \end{vmatrix} \equiv M(\theta)\begin{pmatrix} a \\ b \end{pmatrix}, \tag{12}$$

$x = -\alpha/2 \to 0-$:

$$e\phi(\theta) + f\phi(\theta) = \begin{vmatrix} \psi_1(0-) \\ \psi_2(0-) \end{vmatrix} \equiv M(\theta)\begin{pmatrix} e \\ f \end{pmatrix}. \tag{13}$$

We have defined the 2×2 matrix $M(\theta)$ as

$$M(\theta) = \frac{1}{(2\cosh\theta)^{1/2}} \begin{pmatrix} e^{\theta/2} & e^{-\theta/2} \\ -e^{-\theta/2} & -e^{\theta/2} \end{pmatrix}. \tag{14}$$

Thus,

$$\begin{pmatrix} a \\ b \end{pmatrix} = M^{-1}(\theta) \begin{vmatrix} \psi_1(0+)/\psi_1(0-) & 0 \\ 0 & \psi_2(0+)/\psi_2(0-) \end{vmatrix} M(\theta)\begin{pmatrix} e \\ f \end{pmatrix}$$
$$\equiv N(\theta)\begin{pmatrix} e \\ f \end{pmatrix}. \tag{15}$$

The final matrix $N(\theta)$ is the connection matrix from left to right, and is related to the transmission and reflection amplitudes $T(\theta)$, $R(\theta)$ by

$$N(\theta) = \begin{pmatrix} 1/T(\theta) & R(-\theta)/T(-\theta) \\ R(\theta)/T(\theta) & 1/T(-\theta) \end{pmatrix}. \tag{16}$$

Let us return to Eq. (11), which applies in the interaction region. First, if $v^* = v$ and $v(-x, -x') = v(x, x')$, then

$$\psi_2(x) = \psi_1^*(x) = \psi_1(-x). \tag{17}$$

The symmetry requirements on v are simply time-reversal and parity invariance. Then

$$\psi_1(0+)/\psi_1(0-) = \psi_1(0+)/\psi_1^*(0+) \equiv e^{-i\sigma} \tag{18}$$

and

$$\psi_2(0+)/\psi_2(0-) = \psi_1^*(0+)/\psi_1(0+) = e^{i\sigma}. \tag{19}$$

The function $\sigma(c)$ is a real, odd, analytic, and monotonically increasing function of the potential strength c.

We may easily evaluate

$$N(\theta) = M^{-1}(\theta) \begin{pmatrix} e^{-i\sigma} & 0 \\ 0 & e^{i\sigma} \end{pmatrix} M(\theta)$$
$$= \frac{1}{\sinh\theta} \begin{pmatrix} \sinh(\theta - i\sigma) & -\sinh(i\sigma) \\ \sinh(i\sigma) & \sinh(\theta + i\sigma) \end{pmatrix}, \tag{20}$$

and hence,

$$T(\theta)=\frac{\sinh\theta}{\sinh(\theta-i\sigma)}\,, \tag{21}$$

$$R(\theta)=\frac{\sinh(i\sigma)}{\sinh(\theta-i\sigma)}\,. \tag{22}$$

We will analyze the physics of these amplitudes later, but first let us return to Eq. (11), and consider the two examples to verify our claim that σ is not a universal function of c.

(a) For a potential diagonal in configuration space we choose $v(x,x')=\delta(x-x')v(x)$. If

$$\langle v\rangle \equiv \frac{1}{\alpha}\int_{-\alpha/2}^{\alpha/2} v(x)dx=1,$$

then we have $c=g\alpha$. Thus, Eq. (11) reads

$$\psi_1'=-igv(x)\psi_1 \tag{23}$$

or

$$d\ln\psi_1=-igv(x)dx. \tag{24}$$

Then, integrating from $-\alpha/2$ to $+\alpha/2$,

$$\ln\left(\frac{\psi_1(0+)}{\psi_1(0-)}\right)=-ig\int_{-\alpha/2}^{\alpha/2} v(x)dx=-ic. \tag{25}$$

Thus, we finally arrive at $\sigma=c$.

(b) On the other hand, for a separable potential, we choose $v(x,x')=v(x)v(x')$, $\langle v\rangle=1$, and $c\equiv g\alpha^2$. Equation (11) now reads

$$-i\psi_1'(x)+gv(x)\int_{-\alpha/2}^{\alpha/2} dx'v(x')\psi_1(x')=0. \tag{26}$$

If we define the integral to be η, a constant, then the equation becomes

$$\psi_1'(x)=-ig\eta v(x). \tag{27}$$

$v(x)$ is either even or odd, and thus ψ_1' is either even or odd, so ψ_1 is either odd or even plus a constant β. However, if even, only the constant part β of ψ_1 contributes to the integral η. Thus, we have

$$\psi_1'=-ig\alpha\beta\int_0^x v(x')dx' \tag{28}$$

or

$$\psi_1(\alpha/2)=-ic\beta/2. \tag{29}$$

On the other hand, if $v(x)$ is odd, $\eta=0$, $\psi_1=\beta$, $\psi_1(0+)/\psi_1(0-)=1$, and $\sigma=0$. We now assume $v(x)$ is even. Then,

$$\frac{\psi_1(0+)}{\psi_1(0-)}=\frac{1-ic/2}{1+ic/2} \tag{30}$$

and

$$\sigma=2\tan^{-1}(c/2). \tag{31}$$

We see that (i) σ is not a universal function of c, and (ii) to first order in c, and hence, in the nonrelativistic limit, the two examples agree. It is an easy matter to prove point (ii) for any $v(x,x')$ by iteration of Eq. (11).

To return to Eqs. (21) and (22) for the transmission and reflection amplitudes, we identify the poles, and conclude that bound states occur when $\theta=i\psi_0$, with ψ_0 real and $0<\psi_0<\pi$; and $\psi_0+\sigma=n\pi$, with n an integer. We conclude that there is always exactly one solution and hence, always exactly one bound state. The energy is given by $\omega_0=\cos\psi_0=(-1)^{n+1}\cos\sigma$. If $\sigma=n\pi$, $\omega=\pm1$, then $R=0$, and the potential is transparent at all energies.

We may verify that $d\sigma/dc\leqslant 0$ and thus $d\omega_0/dg\leqslant 0$. Hence, the picture that emerges is that as σ decreases from $n\pi$, a bound state of energy ω_0 emerges from the continuum of positive energy states, passes through zero, and enters the continuum of negative energy states at $\sigma=(n-1)\pi$, just as another bound state once again drops out of the continuum of positive energy states. The system is a periodic function of σ with period 2π, while the bound state energy is a periodic function of period π.

In order to follow explicitly the levels of the continuum, and to examine the possibility of level crossings, it is useful to make the levels discrete by placing the system in a box of length L, and imposing periodic boundary conditions.

Thus, a spinor to the right of the potential a distance $L/2$ is the same as a spinor to the left of the potential a distance $-L/2$. In terms of amplitudes, this translates into

$$\begin{pmatrix} e^{ikL} & 0\\ 0 & e^{-ikL}\end{pmatrix}\begin{pmatrix} a\\ b\end{pmatrix}=\begin{pmatrix} e\\ f\end{pmatrix}, \tag{32}$$

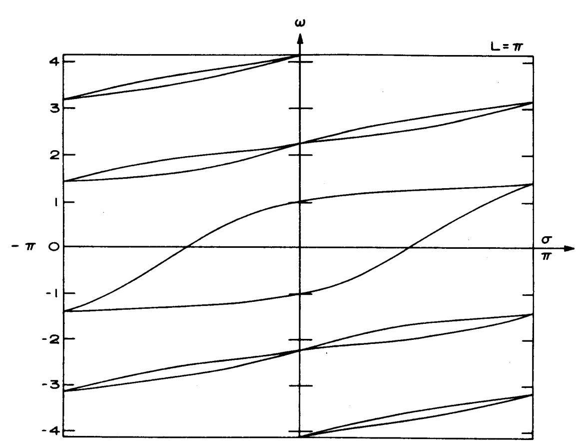

FIG. 1. Energy levels are shown as a function of the renormalized coupling constant σ. We have chosen $L=\pi$.

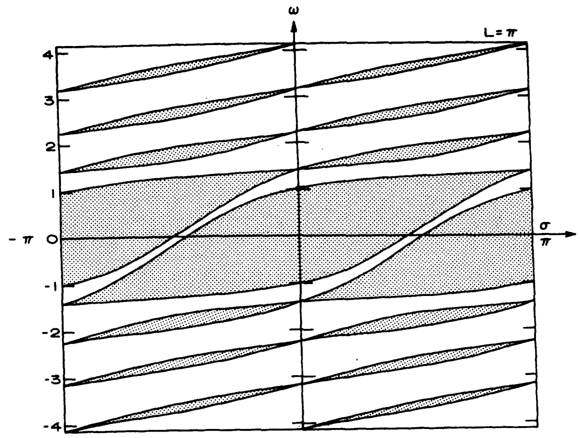

FIG. 2. Band structure of the Dirac-Kronig-Penney model as a function of the renormalized coupling constant σ. We have chosen $L = \pi$.

or using Eq. (15),

$$\begin{pmatrix} e^{ikL} & 0 \\ 0 & e^{-ikL} \end{pmatrix} N(\theta) \begin{pmatrix} e \\ f \end{pmatrix} = \begin{pmatrix} e \\ f \end{pmatrix}. \tag{33}$$

Thus the above matrix must have an eigenvalue of one. But we easily verify that the determinant of the matrix is unity, and hence, both eigenvalues are 1. Thus the trace must be equal to 2. Explicit evaluation gives

$$\tfrac{1}{2}[e^{ikL}\sinh(\theta - i\sigma) + e^{-ikL}\sinh(\theta + i\sigma)] = \sinh\theta. \tag{34}$$

Manipulation puts the equation in the form

$$\pm \frac{k}{(1+k^2)^{1/2}} = \frac{\sin\sigma \sin kL}{1 - \cos kL \cos\sigma},$$
$$\omega = \pm (1+k^2)^{1/2}, \quad 0 \leq k \leq +\infty. \tag{35}$$

Bound states occur for imaginary k, $k = i\kappa$, and then the equation becomes

$$\pm \frac{\kappa}{(1-\kappa^2)^{1/2}} = \frac{\sin\sigma \sin\kappa L}{1 - \cos\sigma \cosh\kappa L},$$
$$\omega = \pm (1-\kappa^2)^{1/2}, \quad 0 \leq \kappa \leq 1. \tag{36}$$

These transcendental equations may be easily solved numerically, and an example is shown in Fig. 1, where we have plotted the energy levels as a function of σ—the coupling constant for a realization of the δ-function potential as a potential diagonal in configuration space. We have taken a typical value $L = \pi$ for the size of the system and followed eight levels over a period 2π of σ. We note the crossing of pairs of levels at $\sigma = n\pi$; the pairs may be classified according to parity $= \pm 1$.

Another amusing way to interpret the results is as a relativistic band problem—the Dirac-Kronig-Penney model. In this case, the potential is an infinite lattice of δ-function potentials of the type we have been considering, with lattice spacing L. The band edges are given by imposing periodic or antiperiodic boundary conditions over a cell. Thus our previous levels are half of the band edges, while the other half of the band edges due to antiperiodic boundary conditions are simply the previous levels at $\sigma + \pi$. Thus the band structure of this model has periodicity π as a function of σ. The bands are shown in Fig. 2, again for the lattice spacing $L = \pi$, as a function of σ over twice a period π. Forbidden bands are shaded, and we note the "valence" band clamping down on the bound state $\omega_0 = \cos\sigma$.

In conclusion, we have exhibited, as promised, ambiguities in the concept of a relativistic δ-function potential. We have not been able to arrive at a reasonable criterion to impose on the limiting procedure to resolve this ambiguity. In fact, one wonders if this ambiguity, which manifests itself in the renormalized strength σ of the δ-function potential being an arbitrary function $\sigma(c)$ of the bare strength c, is not another case which can only be resolved by a fit with the "experiment."

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[1]D. C. Mattis and B. Sutherland, J. Math. Phys. (in press).