

Exact solutions of the Dirac equation with surface delta interactions

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Abstract. The Dirac equation with vector plus scalar surface delta interactions supported by a sphere is exactly solved for all partial waves and parities. Unlike the relativistic one-dimensional delta potentials, surface delta interactions with finite values of the vector and scalar coupling constants require a minimum strength to bind particles. Strong scalar couplings confine relativistic particles at high energies inside the sphere, while the confinement is no longer possible for strong vector potentials. It is also found that the potential causes no effects on the scattering phase shift in the zero-range limit. Therefore, the well known Dirac–Kronig–Penney model in one dimension cannot be generalised to three-dimensional crystal lattices.

1. Introduction

The Fermi contact operator (Fermi 1930) $V(\mathbf{r}) = b\delta(\mathbf{r})$ is usually assumed in perturbative calculations of thermal neutron scattering with solids (Lovesey 1986). Nevertheless, this highly singular operator can only be applied to first order, while second-order perturbation energies diverge. This objection is easily overcome by considering a less singular potential with some fitting parameters. One of these alternative models was introduced by Blinder (1978) who replaced the Fermi contact operator by a surface delta-function potential (SDP) $\delta(r - R)$, i.e. a force field vanishing everywhere except on a spherical shell of radius R . This ‘modified Fermi potential’ leads to an exactly solvable Schrödinger equation for hyperfine interactions (i.e. SDP plus Coulomb potential), in which the nuclear magnetic moment is replaced by a uniformly magnetised spherical shell (Blinder 1978). The SDP plus Coulomb potential also gives closed forms for a large number of parameters appearing in the theory of potential scattering in NN and $N\alpha$ systems (Kok *et al* 1982). Although bound states and resonance properties of SDP have been studied early on (Gottfried 1966, Romo 1973), only recently has the precise mathematical treatment of the non-relativistic Hamiltonian describing a SDP been developed (Antoine *et al* 1987). However, the proper treatment of the Dirac equation for a SDP has not, to the best of our knowledge, even been developed and this problem remains open in the literature.

Although solutions of the Schrödinger equation for such a potential are obtained in a straightforward way, some ambiguities appear in defining the relativistic SDP. Similar problems are found when the one-dimensional Dirac equation is solved for

potentials of different shapes approaching the delta-function limit, since the eigenfunctions approach different values at the interaction point (Sutherland and Mattis 1981). Recently, McKellar and Stephenson (1987a, b) have circumvented this ambiguity in discussing quark-confining properties of nucleons with a Dirac-Kronig-Penney model. They have found boundary conditions for the one-dimensional wavefunction of Dirac particles moving under the action of pure vector and pure scalar sharply peaked potentials. Here vector potential means the time-component of a Lorentz vector while scalar potential means a Lorentz scalar. Hence vector potentials are multiplied by the same Dirac matrix as the particle energy in the wave equation, and scalar potentials could be regarded like a position-dependent mass. Since arbitrarily mixed potentials (vector plus scalar) are often considered in particle physics, the results of McKellar and Stephenson have been generalised recently in order to include such mixed potentials (Domínguez-Adame and Maciá 1989a).

It is our purpose to study the relativistic motion of a particle under the action of vector plus scalar SDPs. We fill the gap that has been left in previous works since we deal with the Dirac equation rather than the Schrödinger equation. Our treatment closely follows the method given by Domínguez-Adame and Maciá (1989a) to solve the one-dimensional Dirac equation for point interaction potentials $V(x) \rightarrow \delta(x)$. First, we introduce a definition of the SDPs which becomes independent of how the delta-function limit is taken, so the above-mentioned ambiguities in defining the relativistic delta interaction are overcome. This potential is one of the most simple two-parameter potentials to be applied in a number of physical problems (see the references of the paper by Antoine *et al* (1987)). These two parameters are the radius of the spherical shell where the force is non-vanishing and the strength of the force; both parameters may be arbitrarily chosen to fit experimental data. Second, we are interested in the bound states (if any) and the scattering states of the Dirac equation for such a potential. Closed formulae for the phase shift and for the scattering amplitude are derived, for all partial waves and spin orientations. Before discussing our conclusions, we study in some detail the confining properties of vector plus scalar SDPs. To be specific, we would like to know if strong SDPs can confine particles inside the sphere or, on the contrary, particles can escape to the outside. This realisation could be interesting in order to improve the quark bag model with abrupt walls, since there exists evidence for quark tunnelling between close nucleons (Goldman and Stephenson 1984, and references therein). Finally, we want to stress that, apart from their purely methodological interest, our results have the virtue of great mathematical simplicity and provide a useful way to study relativistic effects in many other physical situations where short-range interparticle forces are dominant (solid state, molecular and nuclear physics).

2. Relativistic surface delta-function potential

We start with the Dirac equation for a particle in a stationary state of energy E

$$H\Psi = E\Psi. \quad (1)$$

From the Lorentz covariance of the Dirac equation, we can include in the Hamiltonian the time component V of a Lorentz potential and also a Lorentz scalar S potential. Therefore, the Hamiltonian reads ($\hbar = c = 1$).

$$H = \boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta(m + S) + V \quad (2)$$

where

$$\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \quad (3)$$

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \quad (4)$$

in which σ is the vector Pauli spin matrix and I stands for the 2×2 identity matrix. Let V and S be surface delta-function potentials, defined as

$$V(r) = vF_v(r, R) \quad S(r) = sF_s(r, R) \quad (5)$$

v and s being the potential strengths, and $F_v(r, R)$ and $F_s(r, R)$ denoting arbitrary functions of r sharply peaked at R , satisfying the limiting conditions

$$\int_{R^-}^{R^+} dr F_v(r, R) = \int_{R^-}^{R^+} dr F_s(r, R) = 1. \quad (6)$$

Since the potentials are spherically symmetric, the eigenfunctions of definite parity and total angular momentum (J^2, J_z) are written in the form

$$\Psi(r) = \frac{1}{r} \begin{pmatrix} f(r) \\ g(r) \sigma \cdot r/r \end{pmatrix} \Phi_{jm}^l \quad (7)$$

where Φ_{jm}^l are the normalised two-component eigenfunctions of J^2, J_z, L^2 and S^2 (Bjorken and Drell 1964). The radial part of the Dirac equation (1) for the upper $f(r)$ and lower $g(r)$ components of the radial spinor (7) is

$$\begin{aligned} [E + m + S(r) - V(r)]g(r) &= \left(\frac{d}{dr} + \frac{\kappa}{r}\right)f(r) \\ [E - m - S(r) - V(r)]f(r) &= \left(-\frac{d}{dr} + \frac{\kappa}{r}\right)g(r). \end{aligned} \quad (8)$$

Here $\kappa = \mp(j + \frac{1}{2})$ for $l = j \pm \frac{1}{2}$. After rearranging terms, this first-order coupled equation can be written in a closed form as

$$\frac{d}{dr} \begin{pmatrix} f(r) \\ g(r) \end{pmatrix} = \hat{G}(r) \begin{pmatrix} f(r) \\ g(r) \end{pmatrix} \quad (9)$$

$\hat{G}(r)$ being a 2×2 matrix operator expressed in terms of the Pauli matrices as

$$\hat{G}(r) = -\frac{\kappa}{r} \sigma_z + [m + S(r)]\sigma_x - i[E - V(r)]\sigma_y. \quad (10)$$

Equation (9) is solved by a Neumann solution

$$\begin{pmatrix} f(r) \\ g(r) \end{pmatrix} = \hat{P} \exp\left(\int_{r_0}^r dr' \hat{G}(r')\right) \begin{pmatrix} f(r_0) \\ g(r_0) \end{pmatrix} \quad (11)$$

where \hat{P} is the Dyson ordering operator. Considering $r = R^+$ and $r_0 = R^-$ and using (5) and (6), we finally obtain the following boundary conditions (Domínguez-Adame and Maciá 1989a):

$$\begin{pmatrix} f(R^+) \\ g(R^+) \end{pmatrix} = \cos(v^2 - s^2)^{1/2} \begin{pmatrix} 1 & \alpha_- \\ \alpha_+ & 1 \end{pmatrix} \begin{pmatrix} f(R^-) \\ g(R^-) \end{pmatrix} \quad (12)$$

where we have introduced the notation $\alpha_{\pm} = (s \pm v) \tan(v^2 - s^2)^{1/2} / (v^2 - s^2)^{1/2}$, which are always real parameters. Some remarks must be stressed at this point. First, one can easily check that equation (12) reduces to the usual non-relativistic boundary conditions for the SDP (Flügge 1970) in the weak-coupling limit as the particle mass becomes large. However, this assertion is no longer valid for strong coupling, where relativistic treatment is indeed required. On the other hand, boundary conditions become periodic for pure vector SDP ($v \neq 0, s = 0$) since $\alpha_{\pm} = \pm \tan v$, while the periodicity is broken for pure scalar ones ($s \neq 0, v = 0$), where $\alpha_{\pm} = \tanh s$. These differences completely determine the confining properties of vector and scalar SDP. Also note that $|f(R^+)|^2 = |f(R^-)|^2$ and $|g(R^+)|^2 = |g(R^-)|^2$ as $v = n\pi$ and $s = 0$ (here n denotes any arbitrary integer). Therefore, these special values of the vector coupling have no effect on the particle wavefunction, and then the potential becomes transparent to all energies, no matter how strong the interaction is. A similar anomalous behaviour is also found in dealing with one-dimensional vector delta-function potentials (Sutherland and Mattis 1981). Finally, we should comment that the obtained boundary conditions remain valid even if one includes additional potentials in the radial Dirac equation, whenever these potentials are less singular than the SDP at $r = R$.

3. Bound and scattering states

Now we search for the solution of the radial Dirac equation with the boundary conditions given in (12). Without loss of validity, we confine ourselves to positive values of the particle energy throughout this paper. For $r \neq R$ we can decouple equation (8) to obtain

$$g(r) = (E + m)^{-1} \left(\frac{d}{dr} + \frac{\kappa}{r} \right) f(r) \quad r \neq R \quad (13a)$$

$$\frac{d^2 f(r)}{dr^2} + \left(p^2 - \frac{l(l+1)}{r^2} \right) f(r) = 0 \quad r \neq R \quad (13b)$$

where $p = +(E^2 - m^2)^{1/2}$ and we have used the result $\kappa(\kappa + 1) = l(l + 1)$. Solutions of equation (13b) can be written in terms of spherical Bessel and Neumann functions j_l and n_l . Since $f(r)$ must vanish at the origin, we readily find

$$f_{\kappa}(r) = \begin{cases} A_{\kappa} j_l(pr) & r < R \\ j_l(pr) \cos \delta_{\kappa} - n_l(pr) \sin \delta_{\kappa} & r > R \end{cases} \quad (14a)$$

and using the recurrence relations for Bessel and Neumann functions, we have from equation (13a) that

$$g_{\kappa}(r) = (-1)^{j-l+1/2} \left(\frac{p}{E+m} \right) \times \begin{cases} A_{\kappa} j_{l'}(pr) & r < R \\ (j_{l'}(pr) \cos \delta_{\kappa} - n_{l'}(pr) \sin \delta_{\kappa}) & r > R \end{cases} \quad (14b)$$

where $l' = 2j - 1$, A_{κ} is the scattering amplitude and δ_{κ} is the phase shift. The inside and outside solutions are connected through equation (12); one can easily solve for the phase shift and the scattering amplitude to obtain

$$\tan \delta_{\kappa} = \frac{j_l^2[(E+m)/p] \alpha_{+} - j_{l'}^2[p/(E+m)] \alpha_{-}}{-1 + \alpha_{+} j_l n_l[(E+m)/p] - \alpha_{-} j_{l'} n_{l'}[p/(E+m)]} \quad (15)$$

and

$$|A_\kappa|^2 = \frac{[j_l \cos \delta_\kappa - n_l \sin \delta_\kappa][j_{l'} \cos \delta_\kappa - n_{l'} \sin \delta_\kappa]}{\cos^2(v^2 - s^2)^{1/2} \{j_{l'} + (-1)^{j-l+1/2} j_l \alpha_+ [(E+m)/p]\} \times \{j_l + (-1)^{j-l+1/2} j_{l'} \alpha_- [p/(E+m)]\}} \quad (16)$$

where Bessel and Neumann functions are evaluated at pR .

The S -matrix can be directly computed from the scattering phase shift as $S_\kappa = \exp(2i\delta_\kappa) = (1 + i \tan \delta_\kappa)/(1 - i \tan \delta_\kappa)$. Poles of S_κ lying along the positive imaginary axis in the complex p plane will correspond to bound states of the SDP. These poles are given through the following transcendental equation:

$$-q = (m+E)\alpha_+ j_l(iqR) h_l(iqR) + (m-E)\alpha_- j_{l'}(iqR) h_{l'}(iqR) \quad (17)$$

where $q = +(m^2 - E^2)^{1/2}$ and $h_l = j_l + in_l$. This equation has to be solved by the usual search method for any arbitrary value of the angular momentum l . We may ask for the minimum potential 'size' (if any) that can bind at least one state of angular momentum l . The solution to this problem is found by means of the Levinson theorem for Dirac particles (Ma and Ni 1985, Arshansky and Horwitz 1989); the potential possesses n positive bound states whenever $\delta_\kappa(p \rightarrow 0) = n\pi$. On the other hand, an alternative and more explicit way to obtain conditions for particle binding is achieved by expanding equation (17) near $E \approx m$ ($q \rightarrow 0^+$). In so doing, we easily find that the potential parameters must satisfy

$$-\alpha_+/\alpha_- \geq (2l+1)/2mR\alpha_- \quad (18)$$

for binding a particle with energy somewhat below m . This is in contrast to the one-dimensional delta-function potential, where at least one bound state always exists (Domínguez-Adame and Maciá 1989a). One can observe that condition (18) is independent of the value of j , so that the same potential can bind two particles with different j and the same $l = j \pm \frac{1}{2}$. There is a subtlety of condition (18) that we must point out. This condition reduces to $-4mvR \geq 2l+1$ for equally mixed potentials ($\alpha_+ = 2v$, $\alpha_- = 0$), in exact correspondence with the non-relativistic SDP. This result comes from the fact that the Dirac equation reduces to a Schrödinger-like equation for the upper component of the wavefunction when the scalar potential is equal to the vector potential.

Having disposed of the bound states, we now examine the scattering solutions for strong vector and scalar couplings. As mentioned above, these considerations will be useful in studying particle confinement at high energies. To do this, let us start with the scattering amplitude (16) at high energy ($E \sim p$). The numerator is simply written as $\sin(ER + \delta_\kappa - l\pi/2) \sin(ER + \delta_\kappa - l'\pi/2)$, while the denominator becomes

$$j_l j_{l'} [\cos^2(v^2 - s^2)^{1/2} - \sin^2(v^2 - s^2)^{1/2}] + (-1)^{j-l+1/2} [s(j_l^2 + j_{l'}^2) + v(j_l^2 - j_{l'}^2)] \sin[2(v^2 - s^2)^{1/2}] / [2(v^2 - s^2)^{1/2}] \quad (19)$$

with the asymptotic limiting behaviour $j_l(ER) = \sin(ER - l\pi/2)$. Hence the numerator as well as the denominator of the scattering amplitude (16) are smooth functions of the energy as $E \gg m$. It is an easy matter to verify that we can make expression (19) as large as we please whenever $|s| \geq |v|$, so the amplitude of the particle wavefunction inside a sphere of radius R vanishes for strong scalar coupling. On the contrary, expression (19) remains bounded as $|v| > |s|$, even for the limit $v \rightarrow \infty$. The latter is another manifestation of the Klein paradox for strong vector potentials. The relativistic

particle may undergo a tunnelling process from a positive- to a negative-energy state and can go into the sphere. Therefore, concerning confining properties, SDP are quite similar to one-dimensional delta-functions (Domínguez-Adame and Maciá 1989a). We should stress that confining properties do not depend on the sign of the coupling constants at all.

The SDP admits an effective range expansion

$$p \cot \delta_\kappa = -\frac{1}{a_\kappa} + \frac{1}{2} r_\kappa p^2 + \dots \quad (20)$$

where the scattering length a_κ and the effective range r_κ for s states ($\kappa = -1$) are given by

$$a_{-1} = 2mR^2\alpha_+/(1 + 2mR\alpha_+), \quad (21a)$$

$$r_{-1} = (1 + 2mR\alpha_-/3)/8m^3R^2\alpha_+. \quad (21b)$$

For an equally mixed potential ($s = v$) we have $a_{-1} = mR^2v/(1 + mRv)$, which approaches R (hard-sphere limit) as $v \rightarrow \infty$. The scattering length becomes $a_{-1} = 2mR^2/(1 + 2mR)$ for strong scalar coupling, i.e. a hard sphere with an effective radius depending on the particle mass. In the non-relativistic limit, however, a_{-1} approaches the expected value R .

4. Conclusions

Some conclusions may be drawn from the above results. The Dirac equation with vector plus scalar SDP admits exact solutions for all partial waves; boundary conditions are found fully analogous to previous treatments of the one-dimensional relativistic delta-function potentials (Domínguez-Adame and Maciá 1989a). This enables us to study the effects of higher angular momenta on the bound and scattering states. The extension to a superposition of several SDP with different radii and strengths is straightforward; this multisphere potential would admit one positive bound level, provided that the signs of the coupling constants are appropriately chosen and the radii are large enough, for each single SDP entering the potential (Kok *et al* 1982). We have found that SDP requires a minimum 'size' for binding particles, unlike the one-dimensional delta-function potential. In the vanishing-radius limit $R \rightarrow 0$, the SDP has no effect on the phase shift (see equation (10)); therefore, we come to the conclusion that the local function $\delta(r)$ has no sense in three dimensions, according to the suggestion of Avron and Grossmann (1976), so the Dirac-Kronig-Penney model (Domínguez-Adame 1989, and references therein) cannot be generalised to three-dimensional crystals.

In dealing with scattering solutions, we have demonstrated that scalar potentials stronger than (or just equal to) vector potentials act like an impenetrable spherical wall in the infinite-coupling-constant limit, so a particle of any angular momentum inside the sphere will remain there indefinitely. On the contrary, confinement becomes impossible for strong vector coupling due to the Klein paradox. Finally, let us comment that some other potentials could be added to the SDP in straightforward manner since boundary condition (12) still remains valid. In this way, the relativistic singular harmonic-oscillator potential (Domínguez-Adame and Maciá 1989b) in one dimension

is easily generalised to three dimensions, based on the harmonic-oscillator quark model of Ravndal (1982). Consequently, the effects of a short-ranged potential on the relativistic harmonic-oscillator spectroscopy can be exactly evaluated for all partial waves, an interesting result in quark physics at small distances. Also, the model of Kok *et al* (1982) for charge-particle scattering by SDP plus Coulomb potential may be improved using the Dirac equation instead of the Schrödinger equation. Hence relativistic corrections in nuclear reactions involving high-energy particles are easily calculated in a non-perturbative way.

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