Dirac eigenvalues for a softcore Coulomb potential in \( d \) dimensions

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Abstract

A single fermion is bound by a softcore central Coulomb potential \( V(r) = -\frac{v}{(r^d + b)^q}, \quad v > 0, \quad b > 0, \quad q \geq 1, \) in \( d > 1 \) spatial dimensions. Envelope theory is used to construct analytic lower bounds for the discrete Dirac energy spectrum. The results are compared to accurate eigenvalues obtained numerically.

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1. Introduction

For a central potential in \( d \) dimensions the Dirac equation can be written [1] in natural units \( \hbar = c = 1 \) as

\[
i\frac{\partial \Psi}{\partial t} = H \Psi, \quad \text{where} \quad H = \sum_{s=1}^{d} \alpha_s p_s + m \beta + V,
\]

\( m \) is the mass of the particle, \( V \) is a spherically symmetric vector potential, and \( \{\alpha_s\} \) and \( \beta \) are the Dirac matrices which satisfy anti-commutation relations; the identity matrix is implied after the potential \( V \). For stationary states, some algebraic calculations in a suitable basis lead to a pair of first-order linear differential equations in two radial functions \( \{\psi_1(r), \psi_2(r)\} \), where \( r = ||r|| \). For \( d > 1 \), these functions vanish at \( r = 0 \), and, for bound states, they may be normalized by the relation

\[
(\psi_1, \psi_1) + (\psi_2, \psi_2) = \int_0^\infty (\psi_1^2(r) + \psi_2^2(r)) \, dr = 1.
\]

We use inner products \textit{without} the radial measure \( r^{(d-1)} \) because the factor \( r^{(d-1)} \) is already built into each radial function. It has been shown, for example by Jiang [1] (using algebraic ladder-operator methods), that these functions satisfy the following coupled radial equations:

\[
E \psi_1 = (V + m) \psi_1 + (-\partial + k_d/r) \psi_2,
\]

(1)
\[ E\psi_2 = (\partial + k_2/r)\psi_1 + (V - m)\psi_2, \]  

(2)

where \( \partial = \partial/\partial r \), \( k_1 = 0 \), \( k_2 = \tau (j + \frac{d-1}{2}) \), \( d > 1 \), \( \tau = \pm 1 \), and \( j = 1/2, 3/2, 5/2, \ldots \). \( \psi \) is the total angular momentum quantum number. We note that the variable \( \tau \) is sometimes written as \( \omega \), as, for example, in the book by Messiah [2] and the radial functions are often written as \( \psi_1 = \psi \) and \( \psi_2 = F \), as in the book by Greiner [3]. We shall assume that the potential \( V \) is such that there is a discrete eigenvalue \( E \) and that equations (1) and (2) are the eigen-equations for the corresponding radial eigen-states. Our geometrical method (to be outlined below) will also presume that the potential can be written as a smooth transformation \( V(r) = g(-1/r) \), where \( g \) is monotonically increasing and of definite convexity. In this paper we shall present the problem explicitly for the cases \( d > 1 \). We shall label the discrete eigenvalues by \( k_\nu \) and the number \( \nu = \nu_1 \) of nodes in the large radial component \( \psi_1 \). This convenient labeling is suggested by a result of Rose and Newton [4] to the effect that if \( \nu_2 \) is the number of nodes in the small component \( \psi_2 \), then if \( \tau = -1 \), \( \nu_1 = \nu_2 \); and if \( \tau = 1 \), then \( \nu_2 = \nu_1 + 1 \). We study the discrete Dirac spectrum generated by the potential \( V(r) = V_\nu(r) = v f_\nu(r) \), where \( v > 0 \) is the coupling parameter and the potential shape \( f_\nu(r) \) is given by

\[ f_\nu(r) = -\frac{1}{(r^d + br)^{\tau}}. \]

This potential represents a family of softcore (truncated) Coulomb potentials, which are useful as model potentials in atomic and molecular physics. In the limit as \( q \to \infty \), the potential descends to the cut-off Coulomb potential \( f_\infty \) given by

\[ \lim_{q \to \infty} f_\nu(r) = f_\infty(r) = \begin{cases} 
-1/b^\tau & \text{if } r < b; \\
1/r^\tau & \text{if } r \geq b.
\end{cases} \]

The bound states are obtained in terms of three potential parameters: the coupling \( v > 0 \), the cut-off parameter \( b > 0 \), and the power parameter \( q \geq 1 \). The cases \( q = 1 \) and \( 2 \) are of special physical significance [5–13]. The potential \( f_1 \) represents the potential due to a smeared charge and is useful in describing mesonic atoms. The potential \( f_2 \) is similar to the shape of the potential due to a finite nucleus and experienced by the muon in a muonic atom. Extensive applications of the softcore Coulomb potential, \( f_2 \), have been made through model calculations corresponding to the interaction of intense laser fields with atoms [14–19]. The parameter \( b \) can be related to the strength of the laser field, with the range \( b = 20–40 \) covering the experimental laser field strengths [14].

In the non-relativistic case, Mehta and Patil [5] have presented analytical solutions for the \( s \)-state eigenvalues corresponding to the \( f_1 \) potential. Also upper and lower energy bounds and some exact analytic solutions have been found for special cases with the potentials \( f_1 \) and \( f_2 \) [20, 21]. Patil [6] has discussed the analyticity of the scattering phase shifts for two particles interacting through the potentials \( f_\nu \) with \( q = 1 \) and \( q = 2 \). Much less is known concerning the corresponding relativistic problem.

The principal idea that is used in this paper is that of envelope theory. We suppose that a given potential shape \( f(r) \) can be represented as a smooth transformation \( f(r) = g(h(r)) \), where \( h(r) \) is a potential that generates a soluble spectral problem. Since tangents to \( g(h) \) are of the form \( ah(r) + c \), they generate a family of soluble ‘tangential problems’. If the transformation function \( g \) has definite convexity, these tangential problems lead via comparison theorems to a set of energy bounds. Envelope theory picks out the best of these. Although the principal

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1 The Dirac equation for central fields is discussed here.

2 The Dirac equation for the Coulomb central potential is discussed here.
focus of the present paper is on spatial dimensions \( d > 1 \), we note that in \( d = 1 \) dimension, the corresponding potential would be of the form \( V(x) = v f(|x|) \), and the spatial components \( \psi_1(x) \) and \( \psi_2(x) \) of the spinor can be classified as even or odd functions. These components need not now vanish at the origin unless the potential is sufficiently singular there. Meanwhile, the normalization would be given by \( \int_{-\infty}^{\infty} (\psi_1^2(x) + \psi_2^2(x)) \, dx = 1 \). The geometrical reasoning used in the present paper applies equally well to problems in one dimension but, of course, necessitates useful exactly soluble problems to be used as bases for the approximations; the Dirac Coulomb problem, for example, is problematic in \( d = 1 \) dimension \([22, 23]\). Nieto [24] has presented an analysis of non-relativistic problems in \( d \) dimensions, with \( d \) real and positive. For the future, the task of discussing a similar generalization presents itself for relativistic problems and smooth transformations thereof.

In section 2 we review some recent comparison theorems for Dirac eigenvalues and we discuss general scaling and monotonicity properties. In section 3 we describe envelope theory for the Dirac equation and in section 4 we look at the specific case in which the softcore Coulomb potential is written as a smooth convex transformation of a pure Coulomb potential: this generates a simple formula for lower energy bounds. We find some of these bounds explicitly and compare them with accurate values found by direct numerical methods.

2. Comparisons, monotonicity and scaling

It is not a simple matter to characterize the discrete Dirac spectrum variationally \([25–27]\). However, in spite of this, some comparison theorems have recently been proved \([28–30]\) and we state two of these theorems here for use in the present paper.

**Theorem 1** ([28]). The real attractive central potential \( V(r, a) \) depends smoothly on the parameter \( a \) and \( E(a) = E_{k,v}(a) \) is a corresponding discrete Dirac eigenvalue. Then:

\[
\frac{\partial V}{\partial a} \geq 0 \implies E'(a) \geq 0 \quad \text{and} \quad \frac{\partial V}{\partial a} \leq 0 \implies E'(a) \leq 0.
\]

**Theorem 2** ([29]). Suppose that \( E_{k,v}^{(1)} \) and \( E_{k,v}^{(2)} \) are Dirac eigenvalues corresponding to two distinct attractive central potentials \( V^{(1)}(r) \) and \( V^{(2)}(r) \). Then:

\[
V^{(1)}(r) \leq V^{(2)}(r) \implies E_{k,v}^{(1)} \leq E_{k,v}^{(2)}.
\]

If the exact eigenvalues of \( H \) are written \( E(v, b, q, m) \), then we conclude from theorem 1 and the monotone behavior of the potential \( V(r) = v f_0(r) \) with respect to the parameters that these spectral functions are monotone in each parameter, decreasing in \( v \) and \( q \), and increasing in \( b \). Thus:

\[
\frac{\partial E}{\partial v} < 0, \quad \frac{\partial E}{\partial b} > 0 \quad \text{and} \quad \frac{\partial E}{\partial q} < 0.
\]

We now change variable \( r \to \delta r \) in equations (1) and (2), where \( \delta > 0 \) is constant, multiply through by \( \delta \) and compare eigenvalues, we obtain the general scaling law for the family of softcore Coulomb potentials \( V(r) = v f_0(r) \) under the Dirac coupled equations, namely

\[
E(v, b, q, m) = \frac{1}{\delta} E\left(v, \frac{b}{\delta}, q, \delta m\right).
\]

Choosing \( \delta = b \) and \( \delta = 1/m \) we get, respectively, the special scaling laws

\[
E(v, b, q, m) = \frac{1}{b} E(v, 1, q, bm) = mE(v, bm, q, 1).
\]

This much is known in general for the whole class of problems.
3. Envelope theory

Envelope theory has been used since 1980 as a geometrical method of spectral approximation [31–35]. We include here a brief self-contained summary of what is needed for the present task. We consider a potential shape \( f(r) \) that can be written as a smooth transformation \( f(r) = g(h(r)) \) of a potential \( h(r) \) for which the solutions of the Dirac equation are exactly known. In our specific application, \( h(r) \) will be chosen as the Coulomb potential \( h(r) = -1/r \) and \( f(r) = f_0(r) \) is the softcore Coulomb potential, which we are studying. However, it is clearer to discuss the method in general at first. Let us suppose that the transformation function \( g(h) \) is monotonically increasing and convex, that is to say, \( g'(h) > 0 \) and \( g''(h) > 0 \). This means that \( g(h) \) lies above its tangents. If \( r = t \) is the point of contact between curve and tangent, we have (in the convex case) a family of ‘lower’ tangential potentials given by

\[
f(r) \geq f^{(t)}(r) = a(t)h(r) + c(t),
\]

where

\[
a(t) = g'(h(t)) \quad \text{and} \quad c(t) = g(h(t)) - h(t)g'(h(t)).
\]

We note parenthetically that if \( g(h) \) is concave, we obtain, instead, a family of upper bounds. Continuing the convex case, if \( E = D(u) \) describes how a discrete Dirac eigenvalue corresponding to the potential \( uh(r) \) depends on the coupling \( u \), then the potential inequality equation (3) and theorem 2 imply for the original potential \( V(r) = uf(r) \) the spectral inequality

\[
E \geq D(uh(t)) + vc(t).
\]

This expression can then be optimized over the contact point \( t \) to give the lower bound

\[
E(v) \geq E^L(v) = \sup_{t=0} [D(vu(t)) + vc(t)]. \tag{5}
\]

Replacement \( a(t) \) and \( c(t) \), using equation (4), in equation (5) and differentiation with respect to \( h \) gives the value for the critical point \( h = D'(vg'(h)) \). Then we can rewrite the right-hand side of equation (5) by changing the minimization variable from \( t \) to \( u \) by means of the invertible transformation \( u = vg'(h(t)) \), yielding the following alternative form for the best energy bound:

\[
E(v) \geq E^L(v) = \sup_{u=0} [D(u) -uD'(u) + vg(D'(u))]. \tag{6}
\]

4. Energy bounds for the softcore Coulomb potential

We first consider the Dirac equation for the pure Coulomb problem with potential \( V(r) = -u/r \), where the coupling parameter \( u = aZ \) is not too large. We write the exact discrete eigenvalues as \( D_{\nu\psi}(u) = D(u) \) and they are given [1, 22] exactly by

\[
D(u) = m\left[1 + u^2\left(v - (1 - \tau)/2 + \left(k_d^2 - u^2\right)^{1/2}\right)^2\right]^{-\nu/2},
\]

\[
= m\left[1 + u^2\left(n - |k_d| + \left(k_d^2 - u^2\right)^{1/2}\right)^2\right]^{-\nu/2}, \quad 0 < u < 1,
\]

where

\[
k_d = \tau \left( j + \frac{d - 2}{2} \right), \quad \tau = \pm 1,
\]

\( v = 0, 1, 2, \ldots \) is the number of nodes in the upper radial function \( \psi_1(r) \) and \( n \) is the principal quantum number defined in general (for both Coulomb and non-Coulomb central potentials) by

\[
n = v + |k_d| - \frac{1 - \tau}{2}.
\]
Figure 1. The softcore Coulomb potential for $q = 2$ shown with tangential family of shifted Coulomb potentials.

The spectroscopic designation

$$\{s, p, d, \ldots\} \leftrightarrow \ell = \{0, 1, 2, \ldots\}$$

is then provided by the formula

$$\ell = |k_d| - \left(\frac{d - 1}{2}\right).$$
equation (4) are lower bounds to equation (7) and the transformation function 

\[ \mathcal{L} \]

are compared with accurate numerical values \( q = 2 \), \( b = 2 \) and \( v = 58 \) is shown in figure 1.

\[
\nu a(t) < 1 \quad \text{and} \quad a(t) h(r) + b(t)
\]

Since the quantity \(-1/h > 0\), we conclude that \( d\mathcal{E}/dh > 0 \) and \( d^2\mathcal{E}/dh^2 > 0 \). Thus \( g \) is monotonically increasing and convex; its tangents \( f^{(1)}(r) = a(t) h(r) + b(t) \) given by equation (4) are lower bounds to \( f_q(r) \). The case \( q = 2 \), \( b = 2 \) and \( v = 58 \) is shown in figure 1.

Lower energy bounds are therefore provided by equation (6) with \( D(u) \) given by equation (7) and the transformation function \( g \) given explicitly by equation (8). The lower bounds \( \mathcal{E}_{q}^{L} \) are compared with accurate numerical values \( \mathcal{E}_{q} \) in table 1.

The eigenvalue formula equation (7) is based on the Coulomb spectral function \( D(u) \) which admits couplings \( u \) satisfying \( u < 1 \). Thus we require in equation (5) that \( \nu a(t) < 1 \)

\[
\nu a(t) < 1
\]

\[
\nu a(t) < 1
\]

\[
\nu a(t) < 1
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\[
\nu a(t) < 1
\]

\[
\nu a(t) < 1
\]
and consequently we cannot consider arbitrarily large coupling \( v \) for the softcore Coulomb potential. The Coulomb degeneracy \( E_{k,\nu} = E_{-k,\nu+1} \) is expressed by equation (7) and, of course, this symmetry is satisfied by the lower bounds. For instance, from table 1 we see that the lower bounds \( E_{k,\nu} \) are degenerate for the pairs \( \{E_{1,3}, E_{-1,4}\} \) and \( \{E_{3,1}, E_{-3,2}\} \), although the eigenvalues themselves are not exactly equal. Nevertheless, the simple lower bound formula equation (6) is valid for all the discrete Dirac eigenvalues and is often very effective.

5. Conclusion

This paper is based on two ideas: (1) a comparison theorem valid for a discrete Dirac spectrum, and (2) a geometrical theory that generates a family of potentials tangential to a smooth transformation \( g(h) \) of a Dirac-soluble base potential \( h \). These two strands are connected if \( g(h) \) has definite convexity so that its graph lies either above or below its tangents. Meanwhile the tangential potentials are of the form \( ah(r) + c \) and the Dirac equation is soluble exactly for each of them. For given values of the potential parameters, and good quantum numbers, one is then able to find the best tangential potential in the sense of providing the best energy bound. We have used the Coulomb envelope base \( h(r) = -1/r \) to generate optimized energy lower bounds for a family of softcore Coulomb potentials given by \( g(h(r)) = -1/(r^q + b^q)^{3/2} \), where \( b > 0 \) and \( q \geq 1 \). Because the potential is central, the geometric argument leading to the lower bound via the Dirac comparison theorem transcends the question of the number \( d \) of spatial dimensions. The estimate is an energy bound whenever \( g \) has definite convexity.

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