Iterative solutions to the Dirac equation

Hakan Ciftci,[1,3] Richard L. Hall,[1] and Nasser Saad[2]
[1]*Department of Mathematics and Statistics, Concordia University, 1455 de Maisonneuve Boulevard West, Montréal, Québec, Canada H3G 1M8*
[2]*Department of Mathematics and Statistics, University of Prince Edward Island, 550 University Avenue, Charlottetown, Prince Edward Island, Canada C1A 4P3.*
[3]*Fen-Edebiyat Fakültesi, Fizik Bölümü, Gazi Universitesi, 06500 Teknikokullar, Ankara, Turkey*
(Received 7 April 2005; published 1 August 2005)

We consider a single particle which is bound by a central potential and obeys the Dirac equation in d dimensions. We first apply the asymptotic iteration method to recover the known exact solutions for the pure Coulomb case. For a screened Coulomb potential and for a Coulomb plus linear potential with linear scalar confinement, the method is used to obtain accurate approximate solutions for both eigenvalues and wave functions.

DOI: 10.1103/PhysRevA.72.022101 PACS number(s): 03.65.Pm, 31.15.Bs, 31.30.Jv

I. INTRODUCTION

The Dirac equation plays a fundamental role in relativistic quantum mechanics. The equation can be solved exactly for a very few potentials. An early and very detailed analysis of the Dirac spectrum for central potentials has been given by Rose and Newton [1]. The solution for the pure Coulomb field is well known. Exact solutions are known for some other specific cases, such as the Woods-Saxon potential [2]. It is also possible to find classes of exact solutions under very special conditions [3–7]. Unlike the corresponding Schrödinger operator, the Dirac Hamiltonian is not bounded below, and its spectrum cannot be defined variationally. In spite of this it is still possible to find ways to use the variational idea, for example by a saddle-point analysis [8] and by an analysis of the Schrödinger limit in the oscillator basis [9]. Some progress has been made in the establishment of comparison theorems for the Dirac equation without invoking a variational assumption at all [10,11], and this has allowed spectral envelope methods to be used; however, at present, such results apply only to node-free states. Theorems of the Levinson type have now been proved for the Dirac equation in two, three, and d dimensions [12–18]. Solutions of the Dirac equation with shape-invariant potentials have been found by a variety of exact and approximate methods [19–29]. Meanwhile, numerical methods for solving the Dirac equation are continually sought, such as a recent approach by a mapped Fourier grid method [30]. Effective nonvariational approximation methods therefore remain an important area for investigation.

In this paper we first consider the Dirac equation for central potentials in d dimensions. This problem was formulated some decades ago, by Joseph [31]. More recently, Jiang [32], for example, has studied the problem and has obtained a pair of radial equations similar to the well-known case of three dimensions; these equations can be solved exactly for the pure Coulomb field. The d-dimensional angular momentum problem for the Dirac equation has also been studied by group-theoretical methods [33]. We use these results in Sec. II. The main purpose of the present paper is to apply the asymptotic iteration method (AIM) to these central-field problems. The AIM was developed by the present authors [34] for solving second-order linear differential equations, including Schrödinger's. Later the method has been applied to a variety of problems [35–37]. In preparation for the Dirac application, we first extend the method in Sec. III to treat *systems* of homogeneous linear differential equations. In Sec. IV the case of the Dirac Coulomb problem in d dimensions is then treated and solved exactly. In Secs. V and VI we study screened Coulomb problems, and also the linear plus Coulomb potential. For the latter problem, the scalar linear part must dominate the vector linear part in order for discrete eigenvalues to exist [38,39].

II. THE DIRAC EQUATION IN d DIMENSIONS

The Dirac equation for a central field in d dimensions can be written with $\hbar=c=1$ as

$$i\frac{\partial\psi}{\partial t}=H\psi, \quad H=\sum_{j=1}^{d}\alpha_j p_j+\beta[m+U(r)]+V(r), \quad (2.1)$$

where m is the mass of the particle, $V(r)$ is a spherically symmetric vector potential, $U(r)$ is a spherically symmetric scalar potential, and $\{\alpha_j\}$ and β are the usual Dirac matrices satisfying anticommutation relations [the identity matrix is implied after the vector potential term $V(r)$]. After some algebraic calculations (details can be found for example in [32]), one obtains the following first-order linear coupled differential equations:

$$\frac{dG}{dr}=-\frac{k_d}{r}G+[E+m-V(r)+U(r)]F, \quad (2.2)$$

$$\frac{dF}{dr}=-[E-m-V(r)-U(r)]G+\frac{k_d}{r}F. \quad (2.3)$$

These are known as the radial Dirac equations in d dimensions, where $k_d=\tau[j+(d-2)/2]$, and $\tau=\pm1$. We note that the variable τ is sometimes written ω, as, for example, in the book by Messiah [40]. As an example, we suppose that the

particle is moving in a pure vector Coulomb field, that is to say, $V(r)=-A/r$ and $U(r)=0$. In this case Eqs. (2.2) and (2.3) can be written as follows:

$$\frac{dG}{dr} = -\frac{k_d}{r}G + \left(m + E + \frac{A}{r}\right)F, \tag{2.4}$$

$$\frac{dF}{dr} = \left(m - E - \frac{A}{r}\right)G + \frac{k_d}{r}F. \tag{2.5}$$

First of all, we have to obtain some asymptotic forms for $G(r)$ and $F(r)$ functions. At small $r, G(r)$ can be written as the following Euler equation:

$$\frac{d^2G}{dr} = -\frac{1}{r}\frac{dG}{dr} + \left(\frac{k_d^2 - A^2}{r^2}\right)G. \tag{2.6}$$

It is clear that the solution of Eq. (2.6) is $G(r)=r^{\gamma}$, where $\gamma=\sqrt{k_d^2-A^2}$. When a similar analysis at small r is made for $F(r)$, one finds the same general results. At large r, we obtain the following asymptotic differential equation for both $G(r)$ and $F(r)$: $d^2H(r)/dr^2=(m^2-E^2)H(r)$, where $H(r)$ is either $G(r)$ or $F(r)$. We conclude that $H(r)\sim\exp(-r\sqrt{m^2-E^2})$. We therefore adopt the following representations for these radial functions:

$$G(r) = \sqrt{m+E}\,r^{\gamma}\exp(-r\sqrt{m^2-E^2})(\phi_1+\phi_2), \tag{2.7}$$

$$F(r) = \sqrt{m-E}\,r^{\gamma}\exp(-r\sqrt{m^2-E^2})(\phi_1-\phi_2). \tag{2.8}$$

We now substitute these equations into Eqs. (2.4) and (2.5) and use the notation $r=r_1\rho$ to find

$$\frac{d\phi_1}{d\rho} = \left(1 - \frac{a+\gamma}{\rho}\right)\phi_1 - \left(\frac{b+k_d}{\rho}\right)\phi_2, \tag{2.9}$$

$$\frac{d\phi_2}{d\rho} = \left(\frac{b-k_d}{\rho}\right)\phi_1 + \left(\frac{a-\gamma}{\rho}\right)\phi_2, \tag{2.10}$$

where $r_1=1/2\sqrt{m^2-E^2}$, $a=2EAr_1$, and $b=2mAr_1$. It is possible, of course, to solve these equations by using a power series method. However, we shall solve the equations by means of the AIM, which was developed originally for second-order linear differential equations. In the next section, we extend the scope of the AIM to apply to first-order linear coupled differential equations generally; then in Sec. IV we apply the results obtained to the specific Dirac radial equations (2.9) and (2.10) above.

III. ASYMPTOTIC ITERATION METHOD FOR FIRST-ORDER LINEAR COUPLED DIFFERENTIAL EQUATIONS

We consider the following first-order linear coupled differential equations:

$$\phi'_1 = \lambda_0(x)\phi_1 + s_0(x)\phi_2, \tag{3.1}$$

$$\phi'_2 = \omega_0(x)\phi_1 + p_0(x)\phi_2, \tag{3.2}$$

where the prime represents the derivative with respect to x, and $\lambda_0(x), s_0(x), \omega_0(x)$, and $p_0(x)$ are sufficiently differentiable in appropriate domains. If we differentiate Eqs. (3.1) and (3.2) with respect to x, we find that

$$\phi''_1 = \lambda_1(x)\phi_1 + s_1(x)\phi_2, \tag{3.3}$$

$$\phi''_2 = \omega_1(x)\phi_1 + p_1(x)\phi_2, \tag{3.4}$$

where

$$\lambda_1 = \lambda'_0 + \lambda_0^2 + s_0\omega_0,$$

$$s_1 = s'_0 + \lambda_0 s_0 + s_0 p_0,$$

$$\omega_1 = \omega'_0 + \lambda_0\omega_0 + p_0\omega_0,$$

$$p_1 = p'_0 + p_0^2 + s_0\omega_0.$$

Similarly, if we calculate the $(n+2)$th derivative, $n=1,2,\ldots$, we have

$$\phi_1^{(n+2)} = \lambda_{n+1}(x)\phi_1 + s_{n+1}(x)\phi_2, \tag{3.5}$$

$$\phi_2^{(n+2)} = \omega_{n+1}(x)\phi_1 + p_{n+1}(x)\phi_2, \tag{3.6}$$

where

$$\lambda_{n+1} = \lambda'_n + \lambda_n\lambda_0 + s_n\omega_0,$$

$$s_{n+1} = s'_n + \lambda_n s_0 + s_n p_0,$$

$$\omega_{n+1} = \omega'_n + \omega_n\lambda_0 + p_n\omega_0,$$

$$p_{n+1} = p'_n + \omega_n s_0 + p_n p_0.$$

From the ratio of the $(n+2)$th and $(n+1)$th derivatives of ϕ_1 we have

$$\frac{d}{dx}\ln(\phi_1^{(n+1)}) = \frac{\phi_1^{(n+2)}}{\phi_1^{(n+1)}} = \frac{\lambda_{n+1}[\phi_1 + (s_{n+1}/\lambda_{n+1})\phi_2]}{\lambda_n[\phi_1 + (s_n/\lambda_n)\phi_2]}. \tag{3.7}$$

An exactly similar result can be obtained for ϕ_2. However, to solve the system given in Eqs. (3.1) and (3.2), one of these conditions is sufficient. We now introduce the "asymptotic" aspect of the method. If we have, for sufficiently large n,

$$\frac{s_{n+1}}{\lambda_{n+1}} = \frac{s_n}{\lambda_n} := \alpha, \quad n = 1,2,3,\ldots, \tag{3.8}$$

then Eq. (3.7) reduces to $(d/dx)\ln(\phi_1^{(n+1)})=\lambda_{n+1}/\lambda_n$, which yields

$$\phi_1^{(n+1)}(x) = C_1\exp\left(\int^x \frac{\lambda_{n+1}(t)}{\lambda_n(t)}dt\right) = C_1\lambda_n\exp\left(\int^x (\alpha\omega_0 + \lambda_0)dt\right), \tag{3.9}$$

where C_1 is the integration constant. After substituting Eq. (3.9) into $\phi_1^{(n+1)}=\lambda_n(x)\phi_1+s_n(x)\phi_2$, we get

$$\phi_1 + \alpha(x)\phi_2 = C_1 \exp\left(\int^x (\alpha\omega_0 + \lambda_0)dt\right). \quad (3.10)$$

Using Eqs. (3.2) and (3.10) , we can obtain the general solution of $\phi_2(x)$ as follows:

$$\phi_2(x) = \exp\left(\int^x (p_0 - \omega_0\alpha)dt\right)\left\{C_2 + C_1\int^x [\omega_0 \exp\left(\int^t (\lambda_0 - p_0 + 2\omega_0\alpha)d\tau\right)dt]\right\}. \quad (3.11)$$

Once we have obtained $\phi_2(x)$, it is easy to find $\phi_1(x)$ by using one of the coupled equations, or directly from Eq. (3.10).

IV. SOLUTION OF THE DIRAC COULOMB PROBLEM

We now turn back to our first principal application. If we compare Eqs. (2.9) and (2.10) with Eqs. (3.1) and (3.2), we see that $\lambda_0(\rho)=1-(a+\gamma)/\rho$, $s_0(\rho)=-(b+k_d)/\rho$, $\omega_0(\rho)=(b-k_d)/\rho$, and $p_0(\rho)=(a-\gamma)/\rho$. By using our iteration formulas and the iteration termination condition given in Eq. (3.8), we find that $a=\gamma, 1+\gamma, 2+\gamma, \ldots$; this means that $a=n+\gamma$, where $n=0,1,2,\ldots$. In this case b satisfies the following relations:

$$n=0, \quad a=\gamma, \quad b=-k_d,$$

$$n=1, \quad a=1+\gamma, \quad b=-k_d, \quad \pm\sqrt{1+2\gamma+k_d^2},$$

$$n=2, \quad a=2+\gamma, \quad b=-k_d, \quad \pm\sqrt{3+2\gamma+k_d^2}, \quad \pm\sqrt{4+4\gamma+k_d^2},$$

$$n=3, \quad a=3+\gamma, \quad b=-k_d, \quad \pm\sqrt{5+2\gamma+k_d^2}, \quad \pm\sqrt{8+4\gamma+k_d^2}, \quad \pm\sqrt{9+6\gamma+k_d^2}.$$

In general we have, for $a=n+\gamma$, that $b=\pm\sqrt{k_d^2+s(2n-s)+2s\gamma}$, where $s=0,1,2,\ldots,n$. We know from Eqs. (2.9) and (2.10) that $a=2EAr_1$, $b=2mAr_1$, and $r_1=1/2\sqrt{m^2-E^2}$. When we use these equations, we find the following two different expressions for the energy:

$$E = \pm\frac{m}{\sqrt{1+[A/(n+\gamma)]^2}} \quad (4.1)$$

and

$$E = \pm m\sqrt{1-\frac{A^2}{k_d^2+s(2n-s)+2s\gamma}}. \quad (4.2)$$

But these expressions must be equal. From their equality, s must be n or $n+2\gamma$. We know that both n and s are integers, but γ is not an integer, so we find that $s=n$. In this case b becomes $b=\pm\sqrt{k_d^2+n^2+2n\gamma}$, but when $n=0$, b must be $-k_d$. Thus the energy has the form

$$E = \pm m\left[1+\left(\frac{A}{n+\sqrt{k_d^2-A^2}}\right)^2\right]^{-1/2}, \quad (4.3)$$

where we use $\gamma=\sqrt{k_d^2-A^2}$ and $n=0,1,2,3,\ldots$. If we define the principal quantum number as $n_r=n+|k_d|-(d-3)/2=1,2,3,\ldots$, we recover the following well-known formula for the Coulomb energy:

$$E = \pm m\left[1+\left(\frac{A}{n_r-|k_d|+(d-3)/2+\sqrt{k_d^2-A^2}}\right)^2\right]^{-1/2}. \quad (4.4)$$

V. COULOMB WAVE FUNCTIONS

In this section we obtain the Coulomb eigenfunctions by using Eqs. (3.14) and (3.11) . Equation (3.11) includes two independent solutions for $\phi_2(x)$. The first factor of the expression in Eq. (3.11) generally represents the physical solution, so we use this factor as the wave-function generator for our model. If we rewrite this, we have

$$\phi_2(x) = C_2 \exp\left(\int^x (p_0 - \omega_0\alpha)dt\right), \quad (5.1)$$

where C_2 is an integration constant which can be determined by normalization. If we use our iteration procedure, we find the following results for ϕ_2:

$$\phi_2(\rho) = 1, \quad n=0,$$

$$\phi_2(\rho) = -(2\gamma+1)\left(1-\frac{\rho}{2\gamma+1}\right), \quad n=1,$$

$$\phi_2(\rho) = (2\gamma+1)(2\gamma+2)\left(1-\frac{2\rho}{2\gamma+1}+\frac{\rho^2}{(2\gamma+1)(2\gamma+2)}\right), \quad n=2,$$

$$\phi_2(\rho) = -(2\gamma+1)(2\gamma+2)(2\gamma+3)\left(1-\frac{3\rho}{2\gamma+1}+\frac{3\rho^2}{(2\gamma+1)(2\gamma+2)}-\frac{\rho^3}{(2\gamma+1)(2\gamma+2)(2\gamma+3)}\right), \quad n=3.$$

We see from these results that the general formula for $\phi_2(\rho)$ can be written as follows:

$$\phi_2(\rho) = (-1)^n\frac{(2\gamma+n)!}{(2\gamma)!}C_2{}_1F_1(-n,2\gamma+1,\rho), \quad (5.2)$$

where ${}_1F_1$ is the confluent hypergeometric function; since the first argument is a negative integer, the function is a polynomial of degree n. We can now calculate $\phi_1(\rho)$. For this task we use Eq. (3.10), but like $\phi_2(\rho)$, the solution of Eq. (3.10) has two parts. One of them is a polynomial and the other one is an infinite series: we choose the polynomial solution. Thus we find that $\phi_1(\rho)=-\alpha(\rho)\phi_2(\rho)$, where $\alpha(\rho)=s_n/\lambda_n$. If we calculate $\phi_1(\rho)$, using the above equation, we find the following results:

$$\phi_1(\rho) = 0, \quad n=0,$$

TABLE I. Ground-state eigenvalues E for the state $k=-1$, $j=1/2$ (with spectral description $1s_{1/2}$) for the screened Coulomb potential. The energies $(E-1)m_e$, where $m_e=511.004$ keV, are shown, along with corresponding accurate numerical values for comparison.

Z	E	$(E-1)m_e$	Numerical
20	0.991560	−4.3129	−4.3157
30	0.979852	−10.2957	−10.2960
40	0.962675	−19.0732	−19.0732
50	0.939619	−30.8549	−30.8543
60	0.910139	−45.9193	−45.9189
70	0.873475	−64.6548	−64.6545
80	0.828543	−87.6152	−87.6148

$$\phi_1(\rho) = (k_d + b), \quad n = 1,$$

$$\phi_1(\rho) = -(k_d + b)(2\gamma + 1)\left(1 - \frac{\rho}{2\gamma + 1}\right), \quad n = 2,$$

$$\phi_1(\rho) = (k_d + b)(2\gamma + 1)(2\gamma + 2)\left(1 - \frac{2\rho}{2\gamma + 1} + \frac{\rho^2}{(2\gamma + 1)(2\gamma + 2)}\right), \quad n = 3.$$

We conclude from these results that

$$\phi_1(\rho) = (-1)^{n+1}(b + k_d)\frac{(2\gamma + n - 1)!}{(2\gamma)!} C_{21} F_1(1 - n, 2\gamma + 1, \rho), \tag{5.3}$$

where $b=mA/\sqrt{m^2-E^2}$. After obtaining ϕ_1 and ϕ_2, we can recover the radial functions $G(r)$ and $F(r)$ in the well-known form by using Eqs. (2.7) and (2.8). Thus, we have the complete solution of the Dirac equation for the Coulomb problem. In the next sections, we will discuss the solution of the Dirac equation for a screened Coulomb potential and Coulomb plus linear potential with a linear scalar confinement.

VI. DIRAC EQUATION FOR A SCREENED COULOMB POTENTIAL IN THREE DIMENSIONS

In this section we will study a screened Coulomb potential in three dimensions. We use the Mehta and Patil potential [41] which is suitable for large atoms. This potential is defined by

$$V(r) = -\frac{v_1}{r} + \frac{v_2 \lambda}{1 + \lambda r}, \tag{6.1}$$

where $v_1=Z\alpha$, $v_2=(Z-1)\alpha$, and $\lambda=0.98\alpha Z^{1/3}$, and $\alpha \approx 1/137.036$ is the fine-structure constant. For this case, the radial Dirac equations read

$$\frac{dG}{dr} = -\frac{k}{r}G + \left(m + E + \frac{v_1}{r} - W(r)\right)F, \tag{6.2}$$

TABLE II. Eigenvalues E of the Dirac Hamiltonian for the linear plus Coulomb vector potential $V(r)=-A/r+B_1 r$ and a linear scalar potential $U(r)=B_2 r$ in three dimensions, where $A=0.5$, $B_2=0.2$, $B_1=0.1$ The results are given in dimensionless units corresponding to $m=1$. Accurate numerical results E_{num} are shown for comparison; this accuracy was obtained with 20 iterations.

k	n	States	E	E_{num}
−1	0	$1s_{1/2}$	1.25819	1.25819
−1	1	$2s_{1/2}$	1.87575	1.87575
−1	2	$3s_{1/2}$	2.29722	2.29722
1	0	$1p_{1/2}$	1.70367	1.70367
1	1	$2p_{1/2}$	2.15272	2.15272
1	2	$3p_{1/2}$	2.51020	2.51029
−2	0	$2p_{3/2}$	1.74683	1.74683
−2	1	$3p_{3/2}$	2.19096	2.19096
−2	2	$4p_{3/2}$	2.54480	2.54486
2	0	$2d_{3/2}$	2.03889	2.03889
2	1	$3d_{3/2}$	2.41193	2.41193
2	2	$4d_{3/2}$	2.72766	2.72762
−3	0	$3d_{5/2}$	2.04506	2.04506
−3	1	$4d_{5/2}$	2.42019	2.42019
−3	2	$5d_{5/2}$	2.73666	2.73665

$$\frac{dF}{dr} = \left(m - E - \frac{v_1}{r} + W(r)\right)G + \frac{k}{r}F, \tag{6.3}$$

where $W(r)=v_2\lambda/(1+\lambda r)$. The asymptotic behaviors of $F(r)$ and $G(r)$ are the same as for the pure Coulombic potential. For this reason, $G(r)$ and $F(r)$ can be written as follows:

$$G(r) = r^{\gamma}\exp(-r\sqrt{m^2 - E^2})(\phi_1 + \phi_2), \tag{6.4}$$

$$F(r) = r^{\gamma}\exp(-r\sqrt{m^2 - E^2})(\phi_1 - \phi_2), \tag{6.5}$$

where $\gamma=\sqrt{k^2-v_1^2}$. After substituting these forms into into Eqs. (6.2) and (6.3), we have

$$\frac{d\phi_1}{dr} = \left(m + \sigma - \frac{\gamma}{r}\right)\phi_1 - \left(E - W(r) + \frac{v_1 + k}{r}\right)\phi_2, \tag{6.6}$$

$$\frac{d\phi_2}{dr} = \left(E - W(r) + \frac{v_1 - k}{\rho}\right)\phi_1 + \left(\sigma - m - \frac{\gamma}{r}\right)\phi_2, \tag{6.7}$$

where $\sigma=\sqrt{m^2-E^2}$. Now we can use the AIM procedure to obtain the eigenvalues. In preparation for the iteration process it helps first to remove the square-root expression in σ. We do this by the subsitutions

$$\epsilon = \sqrt{\frac{m + E}{m - E}}, \quad \sigma = \frac{2m\epsilon}{1 + \epsilon^2}, \quad E = m\left(\frac{\epsilon^2 - 1}{\epsilon^2 + 1}\right). \tag{6.8}$$

If we use our iteration formulas and the iteration termination condition given in Eq. (3.8), we can construct the following equation, which corresponds to Eq. (3.8):

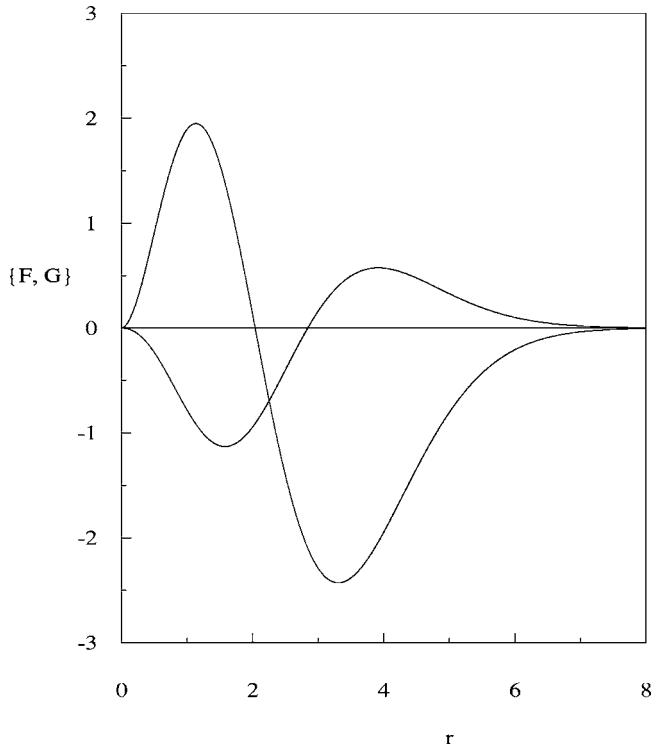

FIG. 1. Dirac radial functions $G(r)$ and $F(r), r>0$, in dimensionless units for $V(r)=-1/2r+0.1r$, $U(r)=0.2r$, $k=-2$, $j=3/2$, $n=2$. This state can be described by the spectroscopic convention as $3p_{3/2}$.

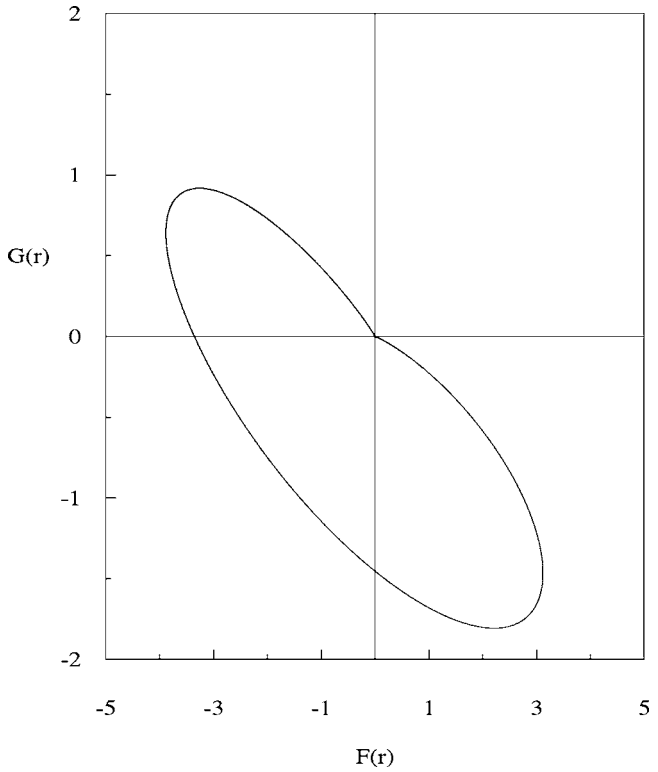

FIG. 2. Dirac spinor orbit $(F(r), G(r)), r>0$, in dimensionless units for the same example as in Fig. 1.

$$\delta(r,\epsilon) = \lambda_{n+1}s_n - s_{n+1}\lambda_n = 0. \tag{6.9}$$

If the problem is exactly solvable, then $\delta(r,\epsilon)=\delta(\epsilon)$ is independent of r and its vanishing gives us the exact results, as with the pure Coulomb problem discussed in Sec. IV. In cases that are not exactly solvable in closed form, $\delta(r,\epsilon)$ depends on both r and ϵ. We then solve the equation $\delta(r_0,\epsilon)=0$ for a suitable fixed $r=r_0$ point, which choice affects the convergence rate of the iteration (this choice is discussed in more detail in the next section). For the problem at hand we chose only one value, $r_0=2$, which fixed choice led to fast convergence in all cases. As the iteration number increases, the eigenvalue estimates become more accurate. The results for the ground-state energies (i.e., for $1s_{1/2}$) with $m=1$ and various atomic numbers Z are presented in Table I. These agree with the results obtained earlier in Ref. [10].

VII. DIRAC EQUATION FOR THE COULOMB PLUS LINEAR POTENTIAL WITH A LINEAR SCALAR TERM

As a further test of the method, we turn in this section to a problem quite different from that of atomic physics: we study the Dirac equation in three dimensions in the case that the vectorial part of the potential is Coulomb plus linear, and the scalar part is linear. We should like to point out that exactly similar calculations can be carried out in arbitrary dimensions d. For this problem the radial Dirac equation is written as follows:

$$\{\vec{\alpha}\cdot\vec{p} + \beta[m+U(r)] + V(r)\}\psi = E\psi, \tag{7.1}$$

where $V(r)=-A/r+B_1r$ and $U(r)=B_2r$, A is positive, and $B_2>B_1$. The correspoding radial Dirac equations become

$$\frac{dG}{dr} = -\frac{k}{r}G + \left(m+E+\frac{A}{r}+(B_2-B_1)r\right)F, \tag{7.2}$$

$$\frac{dF}{dr} = \left(m-E-\frac{A}{r}+(B_2+B_1)r\right)G + \frac{k}{r}F, \tag{7.3}$$

where $k=\tau\left(j+\frac{1}{2}\right)$ and $\tau=\pm1$. Before starting to calculate the energy eigenvalues, we have to consider the asymptotic behavior of $F(r)$ and $G(r)$ at the boundaries. First we consider small r. Since the Coulomb potential dominates in this region, the asymptotic behavior is the same as for the hydrogenic problem: that is to say, $F(r)$ and $G(r)$ behave as r^γ, where $\gamma=\sqrt{k^2-A^2}$. At large r, we find that $H''(r)\sim[2(mB_2+EB_1)r+(B_2^2-B_1^2)r^2]H(r)$, where $H(r)$ is $G(r)$ or $F(r)$. Thus, $H(r)\sim\exp\left(-\alpha r-\frac{1}{2}\beta r^2\right)$, where $\beta=\sqrt{B_2^2-B_1^2}$ and $\alpha=(mB_2+EB_1)/\beta$. Thus we now write $G(r)$ and $F(r)$ in the following way:

$$G(r) = r^\gamma\exp\left(-\alpha r-\frac{1}{2}\beta r^2\right)(\phi_1+\phi_2), \tag{7.4}$$

$$F(r) = r^{\gamma}\exp\left(-\alpha r - \frac{1}{2}\beta r^2\right)(\phi_1 - \phi_2). \tag{7.5}$$

After substituting Eqs. (7.4) and (7.5) into Eqs. (7.2) and (7.3), we find

$$\frac{d\phi_1}{dr} = \left(m + \alpha + (\beta + B_2)r - \frac{\gamma}{r}\right)\phi_1 - \left(E + \frac{A+k}{r} - B_1 r\right)\phi_2, \tag{7.6}$$

$$\frac{d\phi_2}{dr} = \left(E + \frac{A-k}{r} - B_1 r\right)\phi_1 + \left(\alpha - m - \frac{\gamma}{r} + (\beta - B_2)r\right)\phi_2. \tag{7.7}$$

When we compare these equations with Eqs. (3.1) and (3.2) we see that $\lambda_0(r)=m+\alpha+(\eta+B_2)r-\gamma/r$, $s_0(r)=-E-(A+k)/r+B_1 r$, $\omega_0(r)=E+(A-k)/r-B_1 r$, and $p_0(r)=\alpha-m-\gamma/r+(\eta-B_2)r$. We now have to solve $\delta(E,r)=0$ at a suitable r_0 point. Thus r_0 is a parameter of the method. For the present problem, we have found that any r_0 satisfying $1<r_0<3$ is satisfactory in the sense that the iteration sequence converges rapidly. For nonrelativistic problems, we have found earlier that r_0 can be chosen as the peak of a simple scale-optimized trial function; the value of r_0 found in this way for the the ground state is also effective for the excited states. However, since we do not have a suitable variational principle for the Dirac case, the "scale" as represented by r_0, is chosen by the convergence criterion. For the specific example discussed here, we adopted the fixed value $r_0=1.5$ and we obtained E for $A=1/2$, $B_2=0.2$, and $B_1=0.1$. The results are exhibited in Table II (the spectroscopic labeling is explained below). When B_2 is much bigger than B_1, the AIM gives us more accurate results for small iteration numbers, but here, we calculate the energy eigenvalues for rather close values of B_2 and B_1, in order to test the effectiveness of the method.

For the Dirac equation with central potentials l is not a good quantum number. However, a spectroscopic description of the states is still possible if we adopt the following convention [10]. We recall from Sec. II that $\tau=\pm 1$. Meanwhile, the lower index $\ell=0,1,2,\ldots$ of the spherical harmonic Y_ℓ^m appearing [40] in the upper two components of the Dirac four-spinor is related to j by $\ell=j+\frac{1}{2}\tau$, and the parity of the state is given by the formula $P=(-1)^{j+\tau/2}=(-1)^{\ell}$. If the number $n=1,2,3,\ldots$ counts the eigenvalues for each given value of $k=\tau\left(j+\frac{1}{2}\right)$ we may then define the "principal quantum number" for all central potentials as $n_r=n+\ell$. The number ℓ can then be represented by the usual atomic symbol $\{s,p,d,f,\ldots\}$. With this convention we label a state by $n_r D_j$, where $D=s,p,d,f,\ldots$; In the nonrelativistic large-m limit, this notation agrees with the usual Schrödinger description.

VIII. WAVE FUNCTIONS FOR THE LINEAR PLUS COULOMB PROBLEM

It is possible to obtain approximate wave functions for the potential with Coulombic vectorial and scalar linear parts. We calculate the wave functions approximately by using the AIM in the following way. As in Sec. IV, we use the first part of Eq. (3.11) to generate the wave function. In this case, the function $\alpha(r)w_0(r)$ which appears in the wave-function generator cannot be integrated analytically at every iteration, so instead of doing this, we first expand this function near $r=0$ and then integrate the *representation* to give an approximation for $\phi_2(r)$. Once we have $\phi_2(r)$, it is straightforward to obtain $\phi_1(r)$ by using $\phi_1(r)=-\alpha(r)\phi_2(r)$. After obtaining $\phi_1(r)$ and $\phi_2(r)$, we can find $G(r)$ and $F(r)$ by using Eqs. (7.4) and (7.5). Below we give an example of these calculations. We choose the $3p_{3/2}$ state in Table II and find the following corresponding wave functions:

TABLE III. The coefficients a_k and b_k in Eqs. (8.1) and (8.2).

k	a_k	b_k
0	1.7746	−0.22540
1	3.34842	−0.87777
2	2.58401	−1.16405
3	0.89712	−0.79148
4	-4.42384×10^{-2}	−0.30087
5	−0.20572	-4.92821×10^{-2}
6	−0.11569	1.18971×10^{-2}
7	-3.99651×10^{-2}	1.06347×10^{-2}
8	-1.00424×10^{-2}	3.82882×10^{-3}
9	-1.95538×10^{-3}	9.31883×10^{-4}
10	-3.04816×10^{-4}	1.71231×10^{-4}
11	-3.87895×10^{-5}	2.48733×10^{-5}
12	-4.07966×10^{-6}	2.92628×10^{-6}
13	-3.57403×10^{-7}	2.82781×10^{-7}
14	-2.61991×10^{-8}	2.26316×10^{-8}
15	-1.61008×10^{-9}	1.50639×10^{-9}

$$G(r) \approx \left(\sum_{k=0}^{15} a_k r^k\right) r^{0.866\,025}\exp(-2.419\,65r - 0.086\,602\,5r^2), \tag{8.1}$$

$$F(r) \approx \left(\sum_{k=0}^{15} b_k r^k\right) r^{0.866\,025}\exp(-2.419\,65r - 0.086\,602\,5r^2), \tag{8.2}$$

where the a_k and b_k coefficients are given in Table III. We tabulate more coefficients than are needed, in order to demonstrate the stability of the method. In Fig. 1 we show Cartesian plots of the radial functions $G(r)$ and $F(r)$, and in Fig. 2 we exhibit the Dirac spinor orbit [38] defined by $(G(r),F(r)), r\geq 0$. The availability of the wave-function approximations makes these tasks straightforward.

IX. CONCLUSION

In this paper we have shown how the AIM can be used to solve systems of two first-order linear differential equations. In cases where the system represents an eigenvalue problem,

the method yields the eigenfunctions and the eigenvalues. If the exact wave function may be factored in the form of an asymptotic wave function multiplied by a polynomial, the problem can be solved exactly. In other cases, an approximate solution is found by forcing the vanishing of a certain function $\delta(r,E)$ after a finite number of iterations at a fixed expansion point $r=r_0$. The range of values of r_0 which all lead to fast convergence is not narrow: for the problems discussed in this paper the range $1<r_0<3$ was satisfactory; for highly excited states with Coulomb-like potentials, we have found larger values to be better.

In this paper we report applications of the method to bound states of the Dirac equation. First of all, as a test, the known exact solutions of the Coulomb problem in d dimensions were recovered. The method was then applied to find the spectrum and wave functions for a screened Coulomb potential, and also for a very different problem, namely, a linear plus Coulomb potential with a scalar linear confining term. In all cases the method yielded fast convergence to accurate solutions.

ACKNOWLEDGMENTS

Partial financial support of this work under Grants No. GP3438 and No. GP249507 from the Natural Sciences and Engineering Research Council of Canada is gratefully acknowledged by two of us (R.L.H. and N.S., respectively).

[1] M. E. Rose and R. R. Newton, Phys. Rev. **82**, 470 (1951).
[2] P. Kennedy, J. Phys. A **35**, 689 (2002).
[3] J. Franklin, Mod. Phys. Lett. A **14**, 2409 (1999).
[4] A. S. De Castro and J. Franklin, Int. J. Mod. Phys. A **15**, 4355 (2000).
[5] L. Micu, Mod. Phys. Lett. A **18**, 2895 (2003).
[6] S. K. Bose, A. Schulze-Halberg, and M. Singh, Phys. Lett. A **287**, 321 (2001).
[7] S. K. Bose and A. Schulze-Halberg, Mod. Phys. Lett. A **15**, 1583 (2000).
[8] J. Giammarco and J. Franklin, Phys. Rev. A **36**, 5839 (1987).
[9] M. Moshinsky and A. Sharma, J. Phys. A **31**, 397 (1998).
[10] R. L. Hall, Phys. Rev. Lett. **83**, 468 (1999).
[11] G. Chen, Phys. Rev. A **71**, 024102 (2005).
[12] A. Calageracos and N. Dombey, Phys. Rev. Lett. **93**, 180405 (2004).
[13] S. H. Dong, X. W. Hou, and Z. Q. Ma, Phys. Rev. A **58**, 2160 (1998).
[14] Q. C. Lin, Phys. Rev. A **57**, 3478 (1998).
[15] N. Poliatzky, Phys. Rev. Lett. **70**, 2507 (1993).
[16] N. Poliatzky, Phys. Rev. Lett. **76**, 3655 (1996).
[17] Z. Q. Ma, Phys. Rev. Lett. **76**, 3654 (1996).
[18] X. Y. Gu, Z. Q. Ma, and S. H. Dong, Phys. Rev. A **67**, 062715 (2003).
[19] S. H. Dong and Z. Q. Ma, Phys. Lett. A **312**, 78 (2003).
[20] S. H. Dong and M. Lozada-Cossacu, Phys. Lett. A **330**, 168 (2004).
[21] A. D. Alhaidari, Phys. Rev. Lett. **87**, 210405 (2001).
[22] A. D. Alhaidari, Phys. Rev. Lett. **88**, 189901 (2002).
[23] A. D. Alhaidari, J. Phys. A **34**, 9827 (2001).
[24] A. D. Alhaidari, J. Phys. A **35**, 6267 (2002).
[25] J. Y. Gou, X. Z. Fank, and F. X. Xu, Phys. Rev. A **66**, 062105 (2002).
[26] J. Y. Gou, J. Meng, and F. X. Xu, Chin. Phys. Lett. **20**, 602 (2003).
[27] G. Chen, Phys. Lett. A **328**, 116 (2004).
[28] S. H. Dong, J. Phys. A **36**, 4977 (2003).
[29] S. H. Dong, G. H. Sun, and D. Popov, J. Math. Phys. **44**, 4467 (2003).
[30] E. Ackad and M. Horbatsch, J. Phys. A **38**, 3157 (2005).
[31] A. Joseph, Rev. Mod. Phys. **39**, 829 (1967).
[32] Y. Jiang, J. Phys. A **38**, 1157 (2005).
[33] X-Y. Gu *et al.*, Phys. Rev. A **67**, 062715 (2003).
[34] H. Ciftci, R. L. Hall, and N. Saad, J. Phys. A **36**, 11807 (2003).
[35] F. M. Fernandez, J. Phys. A **37**, 6173 (2004).
[36] H. Ciftci, R. L. Hall, and N. Saad, J. Phys. A **38**, 1147 (2005).
[37] T. Barakat, K. Abodayeh, and A. Mukheimer, J. Phys. A **38**, 1299 (2005).
[38] R. L. Hall, J. Math. Phys. **28**, 457 (1987).
[39] R. L. Hall, J. Math. Anal. Appl. **145**, 365 (1990).
[40] A. Messiah, *Quantum Mechanics II* (North-Holland, Amsterdam, 1962). The Dirac equation for central fields is given on p. 928
[41] C. H. Mehta and S. H. Patil, Phys. Rev. A **17**, 34 (1978).