Group theoretic approach for a Dirac particle in Coulomb-like potentials

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Abstract. The energy levels of the Dirac equation with a Kohn–Sham (KS) potential are obtained using algebraic perturbation theory based on the dynamical group structure $SO(2, 1)$ without making any non-relativistic approximation. It has been shown that this formalism reproduces the exact analytical result for the eigenvalues of the Dirac equation with both vector and scalar Coulomb potentials. The lowest-order results obtained from the analytical formulae are found to be in excellent agreement with exact numerical results.

1. Introduction

Exact analytical solutions of Dirac equation with spherically symmetric potentials can be obtained only for a few special cases like the Coulomb potential [1], the Dirac oscillator [2] and for some potentials where the vector and scalar parts are equal and the Dirac equation can be reduced to a solvable Schrödinger equation [3]. Recently various perturbative and other approximation methods [4] have been adopted to obtain Dirac eigenvalues and eigenfunctions, but most of these methods involve either non-relativistic assumptions [5] or lengthy analytic expressions and more computational time.

On the other hand, it has been known that the energy spectra associated with some Hamiltonians can be obtained in a rather simple and elegant way from a knowledge of suitable representations of certain Lie algebras. The algebra used to obtain the eigenvalues and eigenfunctions is referred to as the spectrum generating algebra and the method used is known as dynamical group method [6]. For several interesting applications of this method to non-relativistic quantum mechanics we refer the reader to [7].

For the ordinary relativistic Dirac problem, the application of the dynamical group method was initiated by Barut and Bornzin [8]. (For earlier references on this topic see also [8].) With the help of the tilted state formalism [9] they solved the relativistic Kepler problem for particles with both electric and magnetic charges. The explicit forms of the $O(4, 2)$ algebra and two special $O(2, 1)$ algebras were given by them and a new group theoretical form of the symmetry breaking was pointed out.

In this paper we shall use the Lie algebra of $SO(2, 1)$ group given in [8] together with the variational scaling of the parameter involved, to obtain analytical expressions for the energy values of the Dirac equation with screened Coulomb potentials which are of great importance in a variety of fields such as atomic, nuclear and particle physics. In the following we shall be mainly interested in obtaining the analytical expression for the energy values of the Kohn–Sham (KS) potential which is often utilized in relativistic calculations [10].

This potential has been previously treated by both perturbative [11] and non-perturbative methods [12]. In the former approach the analytical expression obtained for energy values was quite complicated and, in the latter, instead of using the Dirac equation the authors dealt with the Klein–Gordon equation in which a spin–orbit interaction term was included following Papp [13]. However, their formula failed to give satisfactory results in the sense that the contribution from the spin–orbit interaction term was less than that required to explain the actual splitting.

The main motivation of the present work is to overcome the shortcomings of previous approaches and to formulate an elegant algebraic approach exploiting the dynamical symmetry of the problem, without making any non-relativistic approximation. In the following we shall show that group theoretic approach yields a fairly simple analytic formula which will give the energy values with good accuracy (much better than the previous ones). It is worth mentioning that our analytic formula not only reproduces sufficiently accurate energy values for Coulomb plus linear potential [14] but it also gives exact analytic results for a generalized Dirac Coulomb problem involving a Coulomb potential with both Lorentz vector and Lorentz scalar parts [15] obtained in [15] (though, of course, in this case a slightly different representation of the $SO(2, 1)$ algebra is necessary).

The organization of this paper is as follows. In section 2 we shall give the mathematical preliminaries of the $SO(2, 1)$ Lie algebra used in this paper. In section 3 we shall describe the dynamical group method to apply it to KS and other potentials and finally section 4 is kept for discussions and conclusions.

2. Mathematical preliminaries

The $SO(2, 1)$ Lie algebra consists of the three generators T_3, $T_{\pm} = T_1 \pm iT_2$ with the commutation relations

$$[T_+, T_-] = -2T_3, [T_3, T_{\pm}] = \pm T_{\pm} \tag{1}$$

and the Casimir invariant is

$$T^2 = T_3^2 - \tfrac{1}{2}(T_+T_- + T_-T_+). \tag{2}$$

For our purposes, the most useful representation of T_3, T_1, T_2 is the following (see equation (2.31) in [8])

$$T_3 = \frac{1}{2} \left\{ rp^2 + r + \frac{1}{r}(-\alpha^2 - i\alpha\boldsymbol{\alpha} \cdot \hat{r}) \right\}$$

$$T_2 = r \cdot p - i \tag{3}$$

$$T_1 = \frac{1}{2} \left\{ rp^2 - r + \frac{1}{r}(-\alpha^2 - i\alpha\boldsymbol{\alpha} \cdot \hat{r}) \right\}.$$

Here $\alpha \in \mathbb{R}$ will denote, at a later stage, the fine structure constant, $\boldsymbol{\alpha}$ denotes Dirac's matrices (see equation (8)) and $r = |r|$, $\hat{r} = r/r$.

These generators act in the Hilbert space $L^2(\mathbb{R}^3) \times \mathbb{C}^4$ and are self-adjoint not with respect to the usual scalar product of quantum mechanics $\int \psi_1^* \psi_2 \, d^3r$ but with respect to the new scalar product [9]

$$\langle \psi_1 | \psi_2 \rangle = \int \psi_1^* \psi_2 \frac{1}{r} \, d^3r \tag{4}$$

on $L^2(\mathbb{R}^3)$, where $|\psi_1\rangle$ and $|\psi_2\rangle$ are called the group states. This is not the physical scalar product although this can be expressed in terms of the invariant group theoretic product

[16]. These group states are characterized by the principal quantum number n and the total angular momentum j, i.e. $|\psi\rangle = |n, j\rangle$ and they satisfy the orthogonality relation

$$\langle n_1, j_1 | n, j \rangle = \delta n_1, n \delta j_1, j \tag{5}$$

and the completeness relation

$$\sum_{n=j+1}^{\infty} |n, j\rangle\langle n, j| = 1. \tag{6}$$

In the discrete series of representations $D_+^9 \, \alpha^2 \leqslant j(j+1)$, and the Casimir operator T^2 (of equation (7)) is greater than zero. Here the range of values of n and j are given by $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$ and $n = j+1, j+2, \ldots$.

In representation (3) the Casimir operator T^2 is given by [8]

$$T^2 = J^2 - \alpha^2 - i\alpha\boldsymbol{\alpha} \cdot \hat{r} = n'(n'+1) \tag{7}$$

where $\boldsymbol{J} = \boldsymbol{r} \times \boldsymbol{p}$ and n' denoting the eigenvalue of T^2 and is given by equation (12).

Now T^2 can be written as

$$T^2 = \Gamma^2 - \Gamma \tag{8}$$

where the operator

$$\Gamma = \boldsymbol{\sigma} \cdot \boldsymbol{J} + i\alpha\boldsymbol{\alpha} \cdot \hat{r} + 1 \tag{9}$$

has the property that

$$\begin{aligned} \Gamma^2 &= (\boldsymbol{J} + \tfrac{1}{2}\boldsymbol{\sigma})^2 - \alpha^2 + \tfrac{1}{4} \\ &= j(j+1) - \alpha^2 + \tfrac{1}{4} \end{aligned} \tag{10}$$

where $\boldsymbol{\sigma}$ denotes the usual Pauli matrices and j denotes the total angular momentum of the particle.

From equation (10) the eigenvalues of Γ are

$$\gamma = \pm[(j + \tfrac{1}{2})^2 - \alpha^2]^{1/2} \tag{11}$$

and, from equation (7), we get

$$n' = -\gamma \qquad \text{or} \qquad \gamma - 1. \tag{12}$$

If we diagonalize T_3 simultaneously with T^2 (this choice is necessary for a proper description of bound states) then the discrete spectrum of T_3 in the D_+ representation will be given by

$$\bar{n} = \gamma + S \tag{13}$$

where $S = 0, 1, 2, \ldots$.

From equations (7) and (11) it is clear that for n' (which is associated with the Casimir operator T^2) to be real

$$\alpha^2 < (j + \tfrac{1}{2})^2 \tag{14}$$

and then we obtain the D_+ representations of the discrete series of $SO(2, 1)$ which is bounded below.

3. Dynamical group method

The Dirac equation for a central potential $V(r)$ can be written in the form $H_D|\tilde{\Psi}\rangle = E|\tilde{\Psi}\rangle$ where

$$H_D = \alpha \cdot p + \beta m + V(r) \quad (\hbar = c = 1) \tag{15}$$

and $\Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$ with φ and χ are two-component spinors and

$$\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}. \tag{16}$$

$V(r)$ is the potential and E is the energy of the bound electron. For the KS potential [11]

$$V(r) = -\frac{a}{r}[1 + V_1\lambda r + V_2(\lambda r)^2 + V_3(\lambda r)^3] \tag{17}$$

where $a = \alpha Z$ and $\lambda = 1.13\alpha Z^{1/3}$ is a small parameter characterizing the screening (α is the fine structure constant and Z the nuclear charge).

Now the Dirac equation with Hamiltonian (15) and the potential (17) can be put in the following form

$$(\alpha \cdot p + \beta m)|\tilde{\Psi}\rangle = \left(E' + \frac{\alpha}{r} - kr - gr^2\right)|\tilde{\Psi}\rangle \tag{18}$$

where $\alpha = a$, $k = -aV_2\lambda^2$, $g = -aV_3\lambda^3$, $E' = E+\delta$, $\delta = aV_1\lambda$. Without loss of generality we put $\delta = 0$ and henceforth we shall write E instead of E'.

Operating $(\alpha \cdot p + \beta m)$ on both sides of equation (18) from the left and multiplying both sides of the resultant equation by r, we get, after some straightforward calculations,

$$(rp^2 + rm^2)|\tilde{\Psi}\rangle = r\left(E + \frac{\alpha}{r} - kr - gr^2\right)\left(E + \frac{\alpha}{r} - kr - gr^2\right)|\tilde{\Psi}\rangle$$
$$+ \left(i\alpha\frac{\alpha \cdot r}{r} + ikr\alpha \cdot \hat{r} + 2igr^2\alpha \cdot \hat{r}\right)|\tilde{\Psi}\rangle. \tag{18a}$$

Now to relate the Lie algebra (1) to equation (18a), the latter is put into the form [8]

$$\tilde{\Omega}(E)|\tilde{\Psi}\rangle = 0 \tag{18b}$$

where the operator

$$\tilde{\Omega}(E) = rp^2 - r(E^2 - m^2 - 2\alpha k) - \frac{1}{r}(\alpha^2 + i\alpha\alpha \cdot \hat{r}) - i\alpha \cdot \hat{r}kr - 2i\alpha \cdot \hat{r}gr^2$$
$$-2\alpha E + 2Ekr^2 + 2Egr^3 - k^2r^3 - 2gkr^4 - g^2r^5 + 2\alpha gr^2$$
$$= T_3 + \frac{T_+}{2} + \frac{T_-}{2} - (E^2 - m^2 - 2\alpha k)\left(T_3 - \frac{T_+}{2} - \frac{T_-}{2}\right)$$
$$+ \frac{(T^2 - J^2 + \alpha^2)}{\alpha}k\left(T_3 - \frac{T_+}{2} - \frac{T_-}{2}\right) - 2\alpha E$$
$$+ (2Ek + 2\alpha g)\left(T_3 - \frac{T_+}{2} - \frac{T_-}{2}\right)^2 + (2Eg - k^2)\left(T_3 - \frac{T_+}{2} - \frac{T_-}{2}\right)^3$$
$$- 2kg\left(T_3 - \frac{T_+}{2} - \frac{T_-}{2}\right)^4 - g^2\left(T_3 - \frac{T_+}{2} - \frac{T_-}{2}\right)^5$$
$$+ 2\left(\frac{T^2 - J^2 + \alpha^2}{\alpha}\right)g\left(T_3 - \frac{T_+}{2} - \frac{T_-}{2}\right)^2. \tag{19}$$

In equations (18)–(18b) $|\tilde{\psi}\rangle$ denotes the physical state. These physical states $|\tilde{\psi}\rangle$ are normalized and are orthogonal with respect to a different metric. In coordinate space, this amounts to the usual scalar product

$$\langle \tilde{\psi}_1 | r | \tilde{\psi}_2 \rangle = \int \tilde{\psi}_1^* \tilde{\psi}_2 \, d^3 x. \tag{20}$$

Now the tilting transformation is implemented as [9]

$$e^{-i\theta T_2} \tilde{\Omega}(E) e^{i\theta T_2} e^{-i\theta T_2} | \tilde{\psi} \rangle = 0 \tag{21a}$$

so that

$$\tilde{\Omega}(E, \theta) | \Psi \rangle = 0 \tag{21b}$$

where

$$\tilde{\Omega}(E, \theta) = e^{-i\theta T_2} \tilde{\Omega}(E) e^{i\theta T_2}$$

and

$$|\psi\rangle = e^{-i\theta T_2} | \tilde{\Psi} \rangle. \tag{22}$$

The latter is the relation between the group state $|\psi\rangle$ and the physical state $|\tilde{\Psi}\rangle$. Here we use the result that if $H\psi = E\psi$ is an eigenvalue problem, then we can write $H'\psi' = E\psi'$, E being the same in both the cases and where $H' = AHA^{-1}$, $\psi' = A\psi$ (incidentally, $e^{-i\theta T_2}$ is a unitary operator [22].) Therefore, the equivalence of equation (21a) to the original eigenvalue (18b) is obvious. Here θ is allowed to depend on n and j so that the physical state $|\tilde{\psi}\rangle$ is also dependent on n, j and θ.

It follows from the commutation relations (1) that

$$e^{-iT_2\theta} T_3 e^{iT_2\theta} = T_3 \cosh\theta + \left(\frac{T_+}{2} + \frac{T_-}{2} \right) \sinh\theta$$

$$e^{-iT_2\theta} T_+ e^{iT_2\theta} = T_+ \cosh\theta + T_3 \sinh\theta \tag{23}$$

$$e^{-iT_2\theta} T_- e^{iT_2\theta} = T_- \cosh\theta + T_3 \sinh\theta.$$

Using relations (23) in equation (19) we get

$$\begin{aligned}
\tilde{\Omega}(E, \theta) &= T_3 e^\theta + \frac{T_+}{2} e^\theta + \frac{T_-}{2} e^\theta - (E - m^2 - 2\alpha k)e^{-\theta} \left(T_3 - \frac{T_+}{2} - \frac{T_-}{2} \right) \\
&\quad + \left(\frac{T^2 - J^2 + \alpha^2}{\alpha} \right) k e^{-\theta} \left(T_3 - \frac{T_+}{2} - \frac{T_-}{2} \right) \\
&\quad - 2\alpha E + (2Ek + 2\alpha g)e^{-2\theta} \left(T_3 - \frac{T_+}{2} - \frac{T_-}{2} \right)^2 \\
&\quad + (2Eg - k^2)e^{-3\theta} \left(T_3 - \frac{T_+}{2} - \frac{T_-}{2} \right)^3 - 2kg e^{-4\theta} \left(T_3 - \frac{T_+}{2} - \frac{T_-}{2} \right)^4 \\
&\quad - g^2 e^{-5\theta} \left(T_3 - \frac{T_+}{2} - \frac{T_-}{2} \right)^5 \\
&\quad + 2 \left(\frac{T^2 - J^2 + \alpha^2}{\alpha} \right) g e^{-2\theta} \left(T_3 - \frac{T_+}{2} - \frac{T_-}{2} \right)^2.
\end{aligned} \tag{24}$$

Now to obtain the energy values we have to solve the equation

$$\tilde{\Omega}(E, \theta) | \Psi \rangle = 0 \tag{25}$$

$(|\Psi\rangle = |n, j\rangle$ being the group states) which can be written as

$$(\tilde{\Omega}_D(E, \theta) + \tilde{\Omega}_{ND}(E, \theta))|\Psi\rangle = 0 \tag{26}$$

where $\tilde{\Omega}_D(E, \theta)$ and $\tilde{\Omega}_{ND}(E, \theta)$ denote respectively the diagonal and non-diagonal parts respectively of $\tilde{\Omega}(E, \theta)$. By the term diagonal parts of $\tilde{\Omega}(E, \theta)$ we mean the terms involving the operators T_3, T^2, J^2 and powers of them and the constant terms associated with the identity operation in equation (24), because we know that these operators can be simultaneously diagonalized. The other terms in $\tilde{\Omega}(E, \theta)$ are called non-diagonal terms. Specifically, the diagonal terms are

$$\tilde{\Omega}_D(E, \theta) = T_3 e^{\theta} - (E^2 - m^2 - 2\alpha k)T_3 e^{-\theta} + \frac{(T^2 - J^2 + \alpha^2)}{\alpha} ke^{-\theta}T_3$$

$$-2\alpha E + (2Ek + 2\alpha g)e^{-2\theta}\left(\frac{3T_3^2}{2} - \frac{T^2}{2}\right)$$

$$+(2Eg - k^2)e^{-3\theta}(\tfrac{5}{2}T_3^3 - \tfrac{3}{2}T^2 T_3^2 + \tfrac{1}{2}T_3)$$

$$-2kge^{-4\theta}\{\tfrac{35}{8}T_3^4 + \tfrac{25}{8}T_3^2 - \tfrac{15}{4}T^2 T_3^2 + \tfrac{3}{8}(T^2)^2 - \tfrac{3}{4}T^2\}$$

$$-g^2 e^{-5\theta}\{\tfrac{63}{8}T_3^5 + \tfrac{87}{8}T_3^3 + \tfrac{3}{4}T_3 - \tfrac{35}{4}T^2 T_3^3 - \tfrac{19}{4}T^2 T_3 + \tfrac{15}{8}T_3(T^2)^2\}$$

$$+2\left(\frac{T^2 - J^2 + \alpha^2}{\alpha}\right)ge^{-2\theta}\left(\frac{3T_3^2}{2} - \frac{T^2}{2}\right). \tag{26a}$$

Now it is obvious that equation (26) can only be solved perturbatively as it contains the non-diagonal terms. For this purpose an algebraic form of the perturbation theory can be used which was first formulated by Barut and Nagel [20] and later modified by Gerry and Inomata [21]. In this perturbation scheme the non-diagonal terms are treated as small order terms and for a particular n-value, one has to fix the θ-value ($\theta = \theta_n$), because here θ is allowed to depend on n and j. It is then possible to have a closed form normalization for the perturbed states.

The lowest-order approximation to the energy means the energy which is obtained from the following equation [5]

$$\langle n, j|\tilde{\Omega}_D(E, \theta)|n, j\rangle = 0 \tag{26b}$$

which has to be solved to obtain E. As mentioned above higher order corrections to E can be obtained following the scheme of [20, 21]. However, since here we give only the lowest-order results for the energy eigenvalues we skip the details of the higher order calculations.

Now expanding the different powers of $(T_3 - \frac{T_+}{2} - \frac{T_-}{2})$ in equation (24) and using equation (26), we get, after some straightforward algebra,

$$E = \Bigg[-\frac{\alpha}{\bar{n}} + \frac{Ak}{2\bar{n}}e^{-\theta} + \frac{gB}{2\bar{n}}e^{-2\theta} + \left[e^{2\theta}\left(1 + \frac{\alpha^2}{\bar{n}^2}\right) + e^{-\theta}\left\{\left(\frac{\alpha gA + CAg}{\bar{n}}\right) - \frac{\alpha gB}{\bar{n}^2}\right\}\right.$$

$$+e^{-2\theta}\left\{\frac{A^2 k^2}{4\bar{n}^2} - \frac{k^2 B}{2\bar{n}}\right\} + e^{-3\theta}\left\{\frac{Akg B}{2\bar{n}^2} - \frac{kg D}{4\bar{n}}\right\}$$

$$+e^{-4\theta}\left\{\frac{g^2 B^2}{4\bar{n}^2} - \frac{g^2 F}{8\bar{n}}\right\} - \frac{\alpha Ak}{\bar{n}^2} + m^2 + 2\alpha k + Ck\Bigg]^{1/2} \tag{27}$$

where

$$A = 3\bar{n}^2 - (\gamma^2 - \gamma)$$

$$B = 5\bar{n}^3 - 3\bar{n}(\gamma^2 - \gamma) + \bar{n}$$

$$C = \frac{(\gamma^2 - \gamma) - \varkappa(\varkappa + 1) + \alpha^2}{\alpha}.$$

$$D = 35\bar{n}^4 + 25\bar{n}^2 - 30(\gamma^2 - \gamma)\bar{n}^2 + 3(\gamma^2 - \gamma)^2 - 6(\gamma^2 - \gamma)$$

$$F = 63\bar{n}^5 + 87\bar{n}^3 + 6\bar{n} - 70(\gamma^2 - \gamma)\bar{n}^3 - 38\bar{n}(\gamma^2 - \gamma) + 15\bar{n}(\gamma - \gamma)^2 \tag{28}$$

where $\varkappa$ in the expression for C is as follows. $\varkappa$ is the eigenvalue of the operator $1 + \sigma j$. More commonly

$$\varkappa = -1(1+1) \quad \text{if } j = 1 + \tfrac{1}{2}$$
$$= 1 \quad \text{if } j = 1 - \tfrac{1}{2}. \tag{29}$$

It is to be noted that $\varkappa(\varkappa + 1) = 1(1 + 1)$ always holds true. Thus the number 1, i.e. the degree of the ordinary spherical harmonics in terms of which spherical harmonics with spin are expressed is nothing but the azimuthal quantum numbers of Schrödinger theory [18].

Now θ is chosen in such a way that E is minimized i.e.

$$\frac{\mathrm{d}E}{\mathrm{d}\theta} = 0 \qquad \frac{\mathrm{d}^2 E}{\mathrm{d}\theta^2} > 0. \tag{30}$$

This method of treating θ as a variational parameter is just the scaling variational method since T_2 is essentially a generator of scale transformations [19]. It is to be noted that the minimization condition (30) is to be used for each individual energy level. Hence we obtain

$$\left[-\frac{\alpha e^\theta}{\bar{n}} - \frac{Ake^{-\theta}}{2\bar{n}} - \frac{gBe^{-2\theta}}{\bar{n}} \right] \left[e^{2\theta}\left(1 + \frac{\alpha^2}{\bar{n}^2}\right) + e^{-\theta}\left\{ \frac{\alpha gA + CAg}{\bar{n}} - \frac{\alpha gB}{\bar{n}^2} \right\} \right.$$

$$+ e^{-2\theta}\left\{ \frac{A^2 k^2}{4\bar{n}^2} - \frac{k^2 B}{2\bar{n}} \right\} + e^{-3\theta}\left\{ \frac{Akg B}{2\bar{n}^2} - \frac{kg D}{4\bar{n}} \right\}$$

$$\left. + e^{-4\theta}\left\{ \frac{g^2 B^2}{4\bar{n}^2} - \frac{g^2 F}{8\bar{n}} \right\} - \frac{\alpha Ak}{\bar{n}^2} + m^2 + 2\alpha k + Ck \right]^{1/2}$$

$$+ \left[e^{2\theta}\left(1 + \frac{\alpha^2}{\bar{n}^2}\right) - \frac{e^{-\theta}}{2}\left\{ \frac{\alpha gA + CAg}{\bar{n}} - \frac{\alpha gB}{\bar{n}^2} \right\} - e^{-2\theta}\left\{ \frac{A^2 k^2}{4\bar{n}^2} - \frac{k^2 B}{2\bar{n}} \right\} \right.$$

$$\left. - \frac{3}{2}e^{-3\theta}\left\{ \frac{Akg B}{2\bar{n}^2} - \frac{kg D}{4\bar{n}} \right\} - 2e^{-4\theta}\left\{ \frac{g^2 B^2}{4\bar{n}^2} - \frac{g^2 F}{8\bar{n}} \right\} \right] = 0. \tag{31}$$

Equations (27) and (31) together give E' for various values of Z, α, $\varkappa$ and g. We now discuss the following three cases.

3.1. Point Coulomb problem: $V(r) = -\alpha/r$

In this case $\delta = k = g = 0$ in equation (18). Equation (31) gives

$$e^\theta = \frac{m\alpha}{\bar{n}}\frac{1}{\sqrt{1 + \alpha^2/\bar{n}^2}}. \tag{32}$$

so that from equation (27) we get

$$E = \frac{m}{\sqrt{1 + \alpha^2/\bar{n}^2}} \tag{33}$$

which illustrates that our formulae (27) and (31) reproduce exact results for the binding energies of the Coulomb potential.

3.2. Coulomb potential with vector and scalar parts equal to $-\alpha/r$ and $-a/r$ respectively

In this case the Dirac equation is $H|\tilde{\Psi}\rangle = E|\tilde{\Psi}\rangle$ where

$$H = \alpha \cdot p + \beta\left(m - \frac{a}{r}\right) - \frac{\alpha}{r}. \tag{34}$$

We slightly modify the generators of the $SO(2, 1)$ algebra given in (3) in the following way:

$$T_3 = \frac{1}{2}\left[rp^2 + r + \frac{1}{r}\{-\alpha^2 + a^2 - i(\alpha\alpha \cdot \hat{r} - \beta a\alpha \cdot \hat{r})\}\right]$$

$$T_1 = \frac{1}{2}\left[rp^2 - r + \frac{1}{4}\{-\alpha^2 + a^2 - i(\alpha\alpha \cdot \hat{r} - \beta a\alpha \cdot \hat{r})\}\right] \tag{35}$$

$$T_2 = r \cdot p - i$$

and they satisfy the commutation relations given in equation (1). We shall quote in the following the essential steps as the detailed discussion can be found in sections 2 and 3.

The Casimir operator is given by

$$T^2 = J^2 - \alpha^2 + a^2 - i(\alpha - \beta a)\alpha \cdot \hat{r}$$
$$= n'(n' + 1) \tag{36}$$

n' denoting the eigenvalue of T^2 and $n' = -\gamma$ or $\gamma - 1$ where

$$\gamma = \pm[(j + \tfrac{1}{2})^2 - \alpha^2 + a^2]^{1/2}. \tag{37}$$

The eigenvalues of T_3 will be given by

$$\bar{n} = \gamma + S \qquad S = 0, 1, 2, \ldots.$$

In this case equation (24) reads

$$\tilde{\Omega}(E, \theta) = T_1[e^\theta + (E^2 - m^2)e^{-\theta}] + T_3[e^\theta - (E^2 - m^2)e^{-\theta}] - 2\alpha E - 2am. \tag{38}$$

Now choose θ in such a manner that the coefficients of T_1 vanish so that θ is given by

$$e^{2\theta} = m^2 - E^2 \tag{39}$$

and from equation (38) using (39) we get

$$E = \frac{m}{\alpha^2 + \bar{n}^2}\left[\bar{n}\sqrt{\alpha^2 - a^2 + \bar{n}^2} - a\alpha\right]$$

which agrees completely with the results obtained in [15].

Table 1. Potential expansion coefficients from the third-order polynomial least-squares fit to the KS potential with $\lambda = 1.13\alpha Z^{1/3}$ taken from [11].

Z	V_1	V_2	V_3
13	−1.04	0.74	−0.25
30	−1.13	0.91	−0.35
74	−1.21	1.06	−0.43

Table 2. Relativistic binding energies in keV for the KS potential as a function n, x and Z. For comparisons, we also give the results of numerical calculations [11], APT [11] and SLNT [12].

| Z	n		Binding energies in keV				Percentage of errors		
			Numerical	APT	SLNT	Present work	APT	SLNT	Present work
13	1	−1	1.505	1.503	1.471	1.5145	0.1	2.0	0.6
30	1	−1	9.506	9.552	9.469	9.5727	0.5	0.4	0.7
	2	−1	1.157	1.099	1.094	1.1676	5.0	5.0	0.9
		1	1.021	0.9547	1.095	1.0456	7.0	7.0	-2.4
		−2	0.9969	0.9299	0.8619	0.9999	7.0	14.0	0.3
74	1	−1	69.34	70.14	69.90	70.1745	1.0	0.8	1.2
	2	−1	11.96	11.94	11.86	12.0667	0.2	0.8	0.9
		1	11.44	11.46	11.87	11.6236	0.2	4.0	1.6
		−2	10.09	10.05	9.747	10.1675	0.4	3.0	0.8
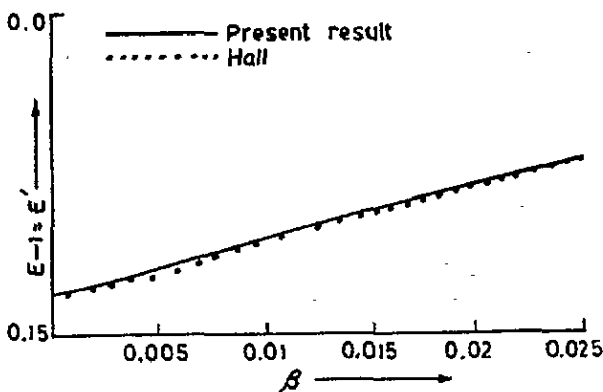
Figure 1. Energy trajectory with $\alpha = 1/2$ and $j = 1/2$.
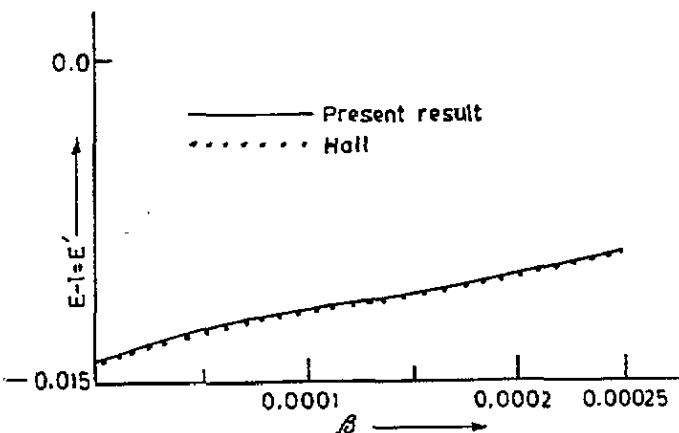

Figure 2. Energy trajectory with $\alpha = 1/2$ and $j = 5/2$.

3.3. Coulomb plus linear potential: $V(r) = -\alpha/r + kr$

In this case $\delta = g = 0$ in equation (18), so that from equation (30) we get

$$\left(-\frac{\alpha e^{\theta}}{\bar{n}} - \frac{Ake^{-\theta}}{2\bar{n}}\right)\left[e^{2\theta}\left(1+\frac{\alpha^2}{\bar{n}^2}\right) + e^{-2\theta}\left(\frac{A^2k^2}{4\bar{n}^2} - \frac{k^2B}{2\bar{n}}\right) - \frac{\alpha Ak}{\bar{n}^2} + Ck + m^2 + 2\alpha k\right]^{1/2}$$

$$+\left[e^{2\theta}\left(1+\frac{\alpha^2}{\bar{n}^2}\right)-e^{-2\theta}\left(\frac{A^2k^2}{4\bar{n}^2}-\frac{k^2B}{2\bar{n}}\right)\right]=0 \tag{41}$$

and equation (27) gives

$$E=-\frac{\alpha e^{\theta}}{\bar{n}}+\frac{Ake^{-\theta}}{2\bar{n}}+\left[e^{2\theta}\left(1+\frac{\alpha^2}{\bar{n}^2}\right)+e^{-2\theta}\left(\frac{A^2k^2}{4\bar{n}^2}-\frac{k^2B}{2\bar{n}}\right)\right.$$
$$\left.-\frac{\alpha Ak}{\bar{n}^2}+Ck+m^2+2\alpha k\right]^{1/2}. \tag{42}$$

Equations (41) and (42) together give the binding energies for α and k.

4. Results and conclusions

In table 1, we give the potential expansion coefficients for a particular value of Z taken from [11]. In table 2, we give the relativistic binding energies obtained from equations (27) and (31) and compare them with the results from analytic perturbation theory (APT) [11], shifted large N technique (SLNT) [12] and numerical calculations [11]. It is evident from the table that our lowest-order analytical results which are simple, in principle, to calculate, are in excellent agreement with the numerical calculations, the maximum error being 2.4%, whereas in the case of APT it is 7% and 14% in SLNT.

In figures 1 and 2 we compare our results obtained from equations (41) and (42) with those from [14] and both the figures indicate that our results reproduce the results of [14] with good accuracy.

So, in this paper, we have succeeded in obtaining compact analytic expressions as well as fairly accurate numerical results for the KS potential and Coulomb plus linear potential. The present method is quite general in the sense that it is applicable to any radially symmetric potential. Moreover, in this approach it is not necessary to reduce the Dirac equation to Schrödinger-like form before applying $SO(2,1)$ formalism.

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References

[1] Bagrov V G, Gitman D M, Ternov I M, Khalilov V P and Shapovalov V N 1977 *Exact Solutions of the Relativistic Wave Equations* (Novosibirsk: Nauka)
[2] Moshinsky M and Szczepaniak A 1989 *J. Phys. A: Math. Gen.* **22** L817
[3] Flügge S 1974 *Practical Quantum Mechanics* vol 1 (Berlin: Springer) p 175
[4] Aharonov Y and Au C K 1979 *Phys. Rev. Lett.* **42** 1582; 1979 *Phys. Rev. Lett.* **43** 176(E); 1980 *Phys. Rev. Lett.* **44** 619(E)
  Au C K and Aharonov Y 1979 *Phys. Rev.* A **20** 2245
  Au C K and Rogers G W 1980 *Phys. Rev.* A **20** 1820
  Sergeev A V and Sherstyuk A I 1984 *Sov. J. Nucl. Phys.* **39** 731
  Rogers G W 1984 *Phys. Rev.* A **30** 35
  Mikhailov A I and Polikanov V S 1968 *Sov. Phys.–JETP* **27** 95
  Rutkowski A 1986 *J. Phys. B: At. Mol. Phys.* **19** 149, 3431
  Nieto M M 1979 *Am. J. Phys.* **47** 1067
  Miramontes J L and Pajares C 1984 *Nuovo Cimento* B **84** 10
  Chatterjee A 1986 *J. Math. Phys.* **27** 2331

Roychoudhury R and Varshni Y P 1987 *J. Phys. A: Math. Gen.* **21** L1083; 1989 *Phys. Rev.* A **39** 5523
Panja M M and Dutt R 1988 *Phys. Rev.* A **38** 3937
Atag S 1989 *J. Math. Phys.* **30** 696
Roy B and Roychoudhury R 1990 *J. Phys. A: Math. Gen.* **23** 3555
Panja M M, Bag M, Dutt R and Varshni Y P 1992 *Phys. Rev.* A **45** 1523
[5] Roy B and Roychoudhury R 1990 *J. Phys. A: Math. Gen.* **23** 5095
[6] Bohm A, Neeman Y and Barut A O (ed) *Dynamical Groups and Spectrum Generating Algebras* vol 1 and 2 (Singapore: World Scientific)
[7] Barut A O 1971 *Dynamical Groups and Generalised Symmetries in Quantum Theory* (Christchurch: University of Canterbury)
Bednar M 1973 *Ann. Phys.* **75** 305
Mathys P and De Meyer H 1988 *Phys. Rev.* A **36** 168 and references therein
[8] Barut A O and Bornzin G L 1971 *J. Math. Phys.* **12** 841
[9] Barut A O 1973 *SIAM J. Appl. Math.* **25** 247
[10] Liberman D, Waber J T and Cromer D T 1965 *Phys. Rev.* **137** A27
[11] McEmnan J, Botto D J, Pratt R H, Bunaciu D and Florescu V 1977 *Phys. Rev.* A **16** 1768
[12] Panja M M, Dutt R and Varshni Y P 1990 *Phys. Rev.* A **42** 106
[13] Papp E 1991 *Ann. Phys., Lpz.* **48** 319
[14] Hall R L 1985 *J. Math. Phys.* **26** 1779
[15] Tutik R S 1992 *J. Phys. A: Math. Gen.* **25** L413
[16] Kleinert H 1968 *Lectures in Theoretical Physics* vol Xb, ed A O Barut and W Brittin (New York: Gordon and Breach)
[17] Gerry C G and Silverman S 1983 *Phys. Lett.* **95A** 481
[18] Fock V A 1978 *Fundamentals of Quantum Mechanics* (Moscow: Mir)
[19] Mitter H and Yamazaki K 1984 *J. Phys. A: Math. Gen.* **17** 1215
[20] Barut A O and Nagel J 1977 *J. Phys. A: Math. Gen.* **10** 1243
[21] Gerry C C and Inomata A 1981 *Phys. Rev.* D **23** 503
[22] Bechler A 1977 *Ann. Phys.* **108** 49