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COMMENT

Dirac equation with Hulthen potential: an algebraic approach

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Abstract. The energy levels of the Dirac equation with scalar and vector Hulthen type potentials are obtained by means of algebraic perturbation calculations which are based upon the dynamical group structure SO(2, 1). Numerical results are given for the particular case when the strengths of the vector and scalar potentials are equal.

1. Introduction

The problem of the screened Coulomb potential is of great importance in all atomic phenomena involving electronic transitions because these potentials are known to describe the effective interaction in many-body atomic phenomena. Since the Schrödinger equation for such a potential does not admit exact solutions except for $l=0$ [1], various approximate methods have been developed [2]. This naïve potential explains quite well the electronic properties of F'—colour centres in alkali halides [3]. Moreover, the model of the three-dimensional delta function could well be considered as a Hulthen potential with the radius of the force going down to zero within a non-relativistic framework [4]. Nevertheless, relativistic effects for a particle under the action of this potential would become important, especially for strong coupling. To the best of our knowledge, the relativistic Hulthen potential has not been treated so far. Recently [5] the existence of bound states for the S-wave Klein-Gordon equation for this type of potential have been shown. In this comment we shall find the energy levels of relativistic Hulthen potential via the SO(2, 1) dynamical group method [6], which has previously been applied mainly to non-relativistic potentials [7].

2. Algebraic formulation

The Dirac equation for a potential with a vector component V and a scalar component V_2 is [8]

$$(W-V)\psi(r)=(\alpha\cdot p)\psi(r)+(m+V_2)\beta\psi(r) \tag{1}$$

where $\psi(r)$ is a four-component wavefunction and W is the relativistic energy (in the units $\hbar=c=1$).

The Dirac equation (1) can be separated in spherical polar coordinates, thereby reducing to a system of two coupled differential equations for the radial wavefunctions

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$F(r)$ and $G(r)$ [9]

$$\frac{\mathrm{d}F}{\mathrm{d}r}-\frac{\chi}{r}F=(V-W+m+V_2)G \tag{2}$$

$$\frac{\mathrm{d}G}{\mathrm{d}r}+\frac{\chi}{r}G=(W-V+m+V_2)F. \tag{3}$$

Here $\chi=-(l+1)$ if the total angular momentum $j=l+\frac{1}{2}$ and $\chi=l$ if $j=l-\frac{1}{2}$. Now eliminating F and writing $W=E+m$, we get from (2) and (3)

$$\frac{\mathrm{d}^2G}{\mathrm{d}r^2}-\frac{\chi(\chi+1)}{r^2}G+(E-V)^2G+2m(E-V)G-V_2(2m+V_2)G$$
$$=\frac{1}{E+2m-V+V_2}\left(-\frac{\mathrm{d}V}{\mathrm{d}r}+\frac{\mathrm{d}V_2}{\mathrm{d}r}\right)\left(\frac{\mathrm{d}G}{\mathrm{d}r}+\frac{\chi}{r}G\right). \tag{4}$$

Now if we put successively

$$G=r\varphi \tag{5}$$

and

$$\varphi=\left(1+\frac{E-V+V_2}{2m}\right)^{1/2}\psi \tag{6}$$

in (4) the resulting equation will be

$$r\frac{\mathrm{d}^2\psi}{\mathrm{d}r^2}+2\frac{\mathrm{d}\psi}{\mathrm{d}r}-\frac{\chi(\chi+1)}{r}\psi+(E-V)^2r\psi+2m(E-V)r\psi-V_2(2m+V_2)r\psi$$
$$=\frac{1}{E+2m-V+V_2}\left(-\frac{\mathrm{d}V}{\mathrm{d}r}+\frac{\mathrm{d}V_2}{\mathrm{d}r}\right)\chi\psi$$
$$+\frac{3}{4}\frac{1}{(E+2m-V+V_2)^2}r\left(-\frac{\mathrm{d}V}{\mathrm{d}r}+\frac{\mathrm{d}V_2}{\mathrm{d}r}\right)^2\psi. \tag{7}$$

We consider vector and scalar Hulthen type potentials which are written as

$$V(r)=-\frac{V_0}{\mathrm{e}^{r/a}-1}\qquad V_2(r)=-\frac{S_0}{\mathrm{e}^{r/a}-1} \tag{8}$$

respectively, where a is the range of the potentials.

Using (8) in (7) yields

$$r\frac{\mathrm{d}^2\psi}{\mathrm{d}r^2}+2\frac{\mathrm{d}\psi}{\mathrm{d}r}-\frac{\chi(\chi+1)}{r}\psi+(E^2+2mE)r\psi$$
$$+\frac{(2EV_0+2mV_0+2mS_0)\,\mathrm{e}^{-r/a}r\psi}{1-\mathrm{e}^{-r/a}}+\frac{(V_0^2-S_0^2)\,\mathrm{e}^{-2r/a}}{(1-\mathrm{e}^{r/a})^2}r\psi$$
$$=\frac{(S_0-V_0)\,\mathrm{e}^{-r/a}}{a[(E+2m)(1-\mathrm{e}^{-r/a})+(V_0-S_0)\,\mathrm{e}^{-r/a}]}\frac{1}{(1-\mathrm{e}^{-r/a})}\chi\psi$$
$$+\frac{3}{4}\frac{(S_0-V_0)^2\,\mathrm{e}^{-2r/a}}{(1-\mathrm{e}^{-r/a})^2}\frac{r\psi}{a^2[(E+2m)(1-\mathrm{e}^{-r/a})+(V_0-S_0)\,\mathrm{e}^{-r/a}]^2}. \tag{9}$$

Note that $\chi(\chi+1) = l(l+1)$, 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 azimathal quantum number of Schrödinger's theory [10].

Now we can take the SO(2, 1) generators for this problem as

$$T_1 = -\frac{1}{2}\left(r\frac{d^2}{dr^2}+2\frac{d}{dr}-\frac{l(l+1)}{r}+r\right). \tag{10}$$

$$T_2 = -i\left(1+r\frac{d}{dr}\right) \tag{11}$$

$$T_3 = -\frac{1}{2}\left(r\frac{d^2}{dr^2}+2\frac{d}{dr}+\frac{l(l+1)}{r}-r\right). \tag{12}$$

T_1, T_2 and T_3 satisfy the following commutation relations:

$$\begin{aligned}[] [T_1, T_2] &= -i\, T_3 \\ [T_2, T_3] &= i\, T_1 \\ [T_3, T_1] &= i\, T_2 \end{aligned} \tag{13}$$

and the Casimir invariant

$$Q = T_3^2 - T_1^2 - T_2^2. \tag{14}$$

Introducing the step operators

$$T_\pm = T_1 \pm i\, T_2 \tag{15}$$

the unitary irreducible representation of SO(2, 1) generated by T_3, $T_\pm$ is given by

$$T_3|l, n\rangle = n|l, n\rangle \tag{16}$$

$$T_{+-}|l, n\rangle = \sqrt{(l+1\pm n)(\pm n - l)}|l, n\pm 1\rangle \tag{17}$$

$$(T_3^2 - T_1^2 - T_2^2)|l, n\rangle = l(l+1)|l, n\rangle \tag{18}$$

where n is the principal quantum number and l is the orbital angular momentum. The states $|\psi\rangle = |l, n\rangle$ are called the group states. Their relation with the physical states will be discussed later on. These group states are actually the basis vectors of the unitary irreducible representation of SO(2, 1).

They satisfy the orthogonality relation

$$\langle n', l'|n, l\rangle = \delta_{l',l}\delta_{n'n} \tag{19}$$

and the completeness relation

$$\sum_{n=l+1} |n, l\rangle\langle n, l| = 1. \tag{20}$$

Now the equation (9) can be expressed with the help of (10)-(12) as

$$\tilde{\Omega}(E)|\tilde{\psi}\rangle = 0 \tag{21}$$

with

$$\begin{aligned}\bar{\Omega}(E)=\{&a^2(E+2m)^2+A\exp[-(T_3-T_1)/a]+B\exp[-2(T_3-T_1)/a]\\&+C\exp[-3(T_3-T_1)/a]+D\exp[-4(T_3-T_1)/a]\}[-(T_3+T_1)\\&+(E^2+2mE)(T_3-T_1)]+\{F\exp[-(T_3-T_1)/a]\\&+G\exp[-2(T_3-T_1)/a]+H\exp[-3(T_3-T_1)/a]\\&-I\exp[-4(T_3-T_1)/a]\}(T_3-T_1)-J\exp[-(T_3-T_1)/a]\chi\\&+K\exp[-2(T_3-T_1)](T_3-T_1)+L\exp[-2(T_3-T_1)/a]\chi\\&+M\exp[-3(T_3-T_1)/a](T_3-T_1)+N\exp[-3(T_3-T_1)/a]\chi\\&+P\exp[-4(T_3-T_1)/a](T_3-T_1)\end{aligned}\tag{22}$$

$$A=2a^2(E+2m)(V_0-S_0-E-2m)-2a^2(E+2m)^2\tag{23}$$

$$B=a^2(E+2m)^2+a^2(V_0-S_0-E-2m)^2-4a^2(E+2m)(V_0-S_0-E-2m)\tag{24}$$

$$C=2a^2(E+2m)(V_0-S_0-E-2m)+2a^2(V_0-S_0-E-2m)^2\tag{25}$$

$$D=a^2(V_0-S_0-E-2m)^2\tag{26}$$

$$F=(2EV_0+2mV_0+2mS_0)a^2(E+2m)^2\tag{27}$$

$$G=(2EV_0+2mV_0+2mS_0)[2a^2(E+2m)(V_0-S_0-E-2m)-a^2(E+2m)^2]\tag{28}$$

$$\begin{aligned}H=(2EV_0+2mV_0+2mS_0)[&a^2(V_0-S_0-E-2m)^2\\&-2a^2(E+2m)(V_0-S_0-E-2m)]\end{aligned}\tag{29}$$

$$I=a^2(2EV_0+2mV_0+2mS_0)(V_0-S_0-E-2m)^2\tag{30}$$

$$J=(S_0-V_0)a(E+2m)\tag{31}$$

$$K=(V_0^2-S_0^2)a^2(E+2m)^2-\tfrac{3}{4}(S_0-V_0)^2\tag{32}$$

$$L=(S_0-V_0)a(E+2m)-(S_0-V_0)a(V_0-S_0-E-2m)\tag{33}$$

$$M=2a^2(V_0^2-S_0^2)(E+2m)(V_0-S_0-E-2m)\tag{34}$$

$$N=(S_0-V_0)a(V_0-S_0-E-2m)\tag{35}$$

$$P=(V_0^2-S_0^2)a^2(V_0-S_0-E-2m).\tag{36}$$

Here $|\bar{\psi}\rangle$ denotes the physical state. Note that in writing (22) we have first multiplied equation (9) on the left by $a^2[(E+2m)(1-e^{-r/a})+(V_0-S_0)\,e^{-r/a}]^2(1-e^{-r/a})^2$.

Next we perform the tilting transformation [11] which is implemented as

$$e^{-i\theta T_2}\bar{\Omega}(E)\,e^{i\theta T_2}\,e^{-i\theta T_2}|\bar{\psi}\rangle=0\tag{37}$$

so that

$$|\psi\rangle=e^{-i\theta T_2}|\bar{\psi}\rangle\tag{38}$$

is the relation between the group state and the physical state. Taking

$$\bar{\Omega}(E,\theta)=e^{-i\theta T_2}\bar{\Omega}(E)\,e^{i\theta T_2}\tag{39}$$

equation (37) can be written as

$$\bar{\Omega}(E,\theta)|\psi\rangle=0.\tag{40}$$

Consequently equation (21) gets transformed into

$$\begin{aligned}
\Bigg\{\Bigg[&-\frac{a^2(E+2m)^2}{w}-\frac{A}{w}\exp\left(-\frac{(T_3-T_1)w}{a}\right)-\frac{B}{w}\exp\left(-\frac{2(T_3-T_1)w}{a}\right)\\
&-\frac{C}{w}\exp\left(-\frac{3(T_3-T_1)w}{a}\right)-\frac{D}{w}\exp\left(-\frac{4(T_3-T_1)w}{a}\right)+(E^2+2mE)w\\
&+Fw\exp\left(-\frac{(T_3-T_1)w}{a}\right)+Gw\exp\left(-\frac{2(T_3-t_1)w}{a}\right)\\
&+Hw\exp\left(-\frac{3(T_3-T_1)w}{a}\right)+Pw\exp\left(-\frac{4(T_3-T_1)w}{a}\right)\\
&-Iw\exp\left(-\frac{4(T_3-T_1)w}{a}\right)+Kw\exp\left(-\frac{2(T_3-T_1)w}{a}\right)\\
&+Mw\exp\left(-\frac{3(T_3-T_1)w}{a}\right)\Bigg]T_3-J\exp\left(-\frac{(T_3-T_1)w}{a}\right)\chi\\
&+L\exp\left(-\frac{2(T_3-T_1)w}{a}\right)\chi+N\exp\left(-\frac{3(T_3-T_1)w}{a}\right)\chi\\
&-\Bigg[\frac{a^2(E+2m)^2}{w}+\frac{A}{w}\exp\left(-\frac{(T_3-T_1)w}{a}\right)+\frac{B}{w}\exp\left(-\frac{2(T_3-T_1)w}{a}\right)\\
&+\frac{C}{w}\exp\left(-\frac{3(T_3-T_1)w}{a}\right)+\frac{D}{w}\exp\left(-\frac{4(T_3-T_1)w}{a}\right)\\
&+(E^2+2mE)w+Fw\exp\left(-\frac{(T_3-T_1)w}{a}\right)+Gw\exp\left(-\frac{2(T_3-T_1)w}{a}\right)\\
&+Hw\exp\left(-\frac{3(T_3-T_1)w}{a}\right)-Iw\exp\left(-\frac{4(T_3-T_1)w}{a}\right)\\
&+Kw\exp\left(-\frac{2(T_3-T_1)w}{a}\right)+Mw\exp\left(-\frac{3(T_3-T_1)w}{a}\right)\\
&+Pw\exp\left(-\frac{4(T_3-T_1)w}{a}\right)\Bigg]T_1\Bigg\}|\psi\rangle=0
\end{aligned}\tag{41}$$

wherein

$$w=\mathrm{e}^{-\theta}.\tag{42}$$

The transformation of equation (41) has been accomplished through the use of the Baker-Hausdorff-Campbell formula:

$$\mathrm{e}^{-\mathrm{i}\theta T_2}(T_3\pm T_1)\,\mathrm{e}^{\mathrm{i}\theta T_2}=\mathrm{e}^{\pm\theta}(T_3\pm T_1).\tag{43}$$

We now use the group states $|\psi\rangle=|l, n\rangle$ and write [6]

$$\langle l, n|\bar{\Omega}(E, \theta)|l, n\rangle=0\tag{44}$$

where $\bar{\Omega}(E, \theta)$ is given by the bracketed portion of equation (41).

A method of obtaining in closed form the matrix elements of the exponential operator of equation (41) in the SO(2, 1) group state basis has been established by Bargmann [12]. The application of this method yields

$$\langle n'l|\exp\left(-\frac{(T_3-T_1)w}{a}\right)|n,l\rangle = A_{n'n}\left(1+\frac{w}{2a}\right)^{-n'-n}\left(\frac{w}{2a}\right)^{n'-n} 2F_1\left(l+1-n,-n-l,1+n'-n,\frac{w^2}{4a^2}\right) \qquad n'\geqslant n \tag{45}$$

$$\langle n'l|\exp\left(-\frac{2(T_3-T_1)w}{a}\right)|n,l\rangle = A_{n'n}\left(1+\frac{w}{a}\right)^{-n'-n}\left(\frac{w}{a}\right)^{n'-n} 2F_1\left(l+1-n,-n-l,1+n'-n,\frac{w^2}{a^2}\right) \qquad n'\geqslant n \tag{46}$$

$$\langle n'l|\exp\left(-\frac{3(T_3-T_1)w}{a}\right)|n,l\rangle = A_{n'n}\left(1+\frac{3w}{2a}\right)^{-n'-n}\left(\frac{3w}{2a}\right)^{n'-n} 2F_1\left(l+1-n,-n-l,1+n'-n,\frac{9w^2}{4a^2}\right) \qquad n'\geqslant n \tag{47}$$

$$\langle n'l|\exp\left(-\frac{4(T_3-T_1)w}{a}\right)|n,l\rangle = A_{n'n}\left(1+\frac{2w}{a}\right)^{-n'-n}\left(\frac{2w}{a}\right)^{n'-n} 2F_1\left(l+1-n,-n-l,1+n'-n,\frac{4w^2}{a^2}\right) \qquad n'\geqslant n \tag{48}$$

where

$$A_{n'n}=\frac{1}{\Gamma(n'-n+1)}\left(\frac{\Gamma(n'-l)\Gamma(n'+l+1)}{\Gamma(n-l)\Gamma(n+l+1)}\right)^{1/2} \qquad n'\geqslant n. \tag{49}$$

The function $2F_1(a,b,c;Z)$ is the Gauss hypergeometric function [13] which in (45)-(48) always reduces to a polynomial. Finally, the matrix elements of the energy functional $\bar{\Omega}(E,\theta)$ can be calculated on account of the completeness relation (20) for the SO(2, 1) group states. Hence using equations (16)-(18) and (45)-(49) in equation (44) one can get the energy $E^{(0)}_{n,l}$ by solving the latter equation. However, the solution being θ dependent, it has been shown by Feranchuk and Komarov [14] that the choice

$$\left.\frac{\mathrm{d}E^{(0)}_{n,l}(\theta)}{\mathrm{d}\theta}\right|_{\theta=\theta_{nl}}=0 \tag{50}$$

$$\left.\frac{\mathrm{d}^2E^{(0)}_{nl}(\theta)}{\mathrm{d}\theta^2}\right|_{\theta=\theta_{nl}}>0 \tag{51}$$

yields attractive results for the approximations of zeroth order. 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. This has the added advantage that the lowest approximation satisfies both the virial theorem and the Hellmann-Feynman theorem [15]. Equations (44) and (50) together give $E_{nl}^{(0)}(\theta)$ for various values of $1/a$.

3. Numerical results and discussions

Here we apply the results of section 2 to the particular case when $V_0 = S_0$ in equation (8). This has been done to compare a part of our results with exact results. It is well known that when $V_0 = S_0$ the Dirac equation reduces to the Schrödinger equation and the S-wave eigenvalues for Hulthen potential can be calculated exactly [1]. In table 1, we list the eigenvalues $E_{nl}^{(0)}$ of 1S, 2S, 3S, 2P, 3P and 3D states and for various values of $\lambda = 1/a$. The 1S, 2S and 3S results are compared with the exact results obtained from Schrödinger theory. It is evident from the table that the agreement is good considering the fact that no higher-order correction has been taken into account (except for the 3S case for $\lambda = 0.2$). It is expected that higher-order corrections would be significant for higher n values. Also it should be mentioned here that this method is general enough to be applicable to any potential with a vector and scalar part.

Table 1. Spin averaged eigenvalues $E_{nl}^{(0)}$ for the Hulthen potential whose vector and scalar components are identical and are given by $V_V = V_S = -V_0/(e^{r/a} - 1)$ (taking $m = V_0 = 1$). In parantheses are given for an S-state, the exact energy value.

$\lambda = 1/a$	1S	2S	3S
0.2	−1.9057	−1.6708	−1.3768
	(−1.8881)	(−1.6)	(−1.2371)
0.1	−1.9758	−1.9078	−1.8033
	(−1.9860)	(−1.8881)	(−1.7600)
0.05	−1.9939	−1.9763	−1.9474
	(−1.9927)	(−1.9712)	(+1.9359)
0.02	−1.9990	−1.9962	−1.9914
	(−1.9988)	(−1.9953)	(−1.9895)

$\lambda = 1/a$	2P	3P	3D
0.2	−1.6296	−1.2640	−1.2704
0.1	−1.8964	−1.6424	−1.7712
0.05	−1.9733	−1.6808	−1.9389
0.02	−1.9957	−1.6936	−1.9902

References

[1] Flugge S 1974 *Practical Quantum Mechanics* vol 1 (Berlin: Springer) p 175
[2] Roy B and Roychoudhury R 1987 *J. Phys. A: Math. Gen.* **20** 3051
Sever R and Tezcan C 1987 *Phys. Rev.* A **36** 1045

de Meyer H, Fack and Vanden Berghe G 1985 *J. Phys. A: Math. Gen.* **18** L849
Popov V S and Weinberg V M 1985 *Phys. Lett.* **107A** 371
Patil S H 1984 *J. Phys. A: Math. Gen.* **17** 575
[3] Berezin A A 1972 *Phys. Stat. Sol.* b **50**; 1979 *J. Phys. C: Solid State Phys.* **12** L363
[4] Berezin A A 1986 *Phys. Rev.* B **33** 2122
[5] Dominguez Adame F 1989 *Phys. Lett.* **136A** 175
[6] Barut A O 1971 *Dynamical Group and Generalized Symmetries in Quantum Theory* (Christchurch: University of Canterbury Press)
[7] Matthys P and De Meyer H 1988 *Phys. Rev.* A **36** 168
[8] Rein D W 1977 *Nuovo Cimento* A **38** 19
[9] Bethe H A and Salpater E E 1957 *Quantum Mechanics of One and Two Electron Atoms* (Berlin: Springer)
[10] Fock V A 1978 *Fundamentals of Quantum Mechanics* (Moscow: Mir)
[11] Barut A O 1973 *SIAM J. Appl. Maths.* **25** 247
[12] Bargmann V 1947 *Ann. Math.* **48** 568
[13] Abramowitz M and Stegun I A 1964 *Handbook of Mathematical Functions* (Washington DC: US Government Printing Office)
[14] Feranchuk I D and Komarov L I 1982 *Phys. Lett.* **88A** 211
[15] Mitter H and Yamazaki K 1984 *J. Phys. A: Math. Gen.* **17** 1215