Vol 12 No 10, October 2003
1009-1963/2003/12(10)/1054-04

Chinese Physics

© 2003 Chin. Phys. Soc.
and IOP Publishing Ltd

Bound states of the Klein–Gordon and Dirac equations for potential $V(r) = Ar^{-2} - Br^{-1}$

Qiang Wen-Chao(强稳朝)

Faculty of Science, Xi'an University of Architecture and Technology, Xi'an 710055, China

(Received 24 January 2003; revised manuscript received 16 June 2003)

The exact normalized bound-state wavefunctions and energy equations of Klein–Gordon and Dirac equations are given with equal scalar and vector potentials $s(r) = v(r) = V(r)/2 = (Ar^{-2} - Br^{-1})/2$.

Keywords: Coulomb potential, inverse square potential, Klein–Gordon equation, Dirac equation, bound-state

PACC: 0300, 0365

1. Introduction

It is well known that when a particle moves in a strong potential field the relativistic quantum mechanics can give more precise result than the non-relativistic quantum mechanics. Perhaps owing to the difficulties in mathematics, except for a few examples, such as the hydrogen atom and electrons in a uniform magnetic field, the problems that can be exactly solved in relativistic quantum mechanics for Klein–Gordon or Dirac equations are seldom. In recent years, some authors have assumed the equality of scalar potential and vector potential and solved the Klein–Gordon, as well as Dirac, equations for some typical potential fields.[1−4] We have also solved the Klein–Gordon and Dirac equations for the equal scalar and vector harmonic oscillator potentials, and obtained a non-s-wave solution, but not the exact solution of a relativistic harmonic oscillator.[5] We have also solved the Klein–Gordon equation for a ring-shaped harmonic oscillator potential.[6] In this paper, we shall solve the Klein–Gordon and Dirac equations for a combined potential of a Coulomb and an inverse square potentials.[7−9] This potential can describe the electrons in the outer shell of an alkaline metal atom.[8,9] We will present the normalized wavefunctions and energy equation, in the next sections.

2. Bound-state solution of the Klein–Gordon equation with scalar and vector potentials equal to each other

According to Ref.[10], the Klein–Gordon equation for equal scalar and vector potentials is ($\hbar = c = 1$)

$$\left[\boldsymbol{P}^2 - \left(E - \frac{V(r)}{2}\right)^2\right]\psi = -\left(\mu + \frac{V(r)}{2}\right)^2\psi, \tag{1}$$

where $\boldsymbol{P}$ is the momentum operator, E and μ are the energy and rest mass of the particle respectively. For the potential[7−9]

$$V(r) = \frac{A}{r^2} - \frac{B}{r}, \tag{2}$$

in spherical coordinates, the radial part of Eq.(1) is

$$\frac{1}{r}\frac{\partial^2}{\partial r^2}(rR(r)) - \left[\frac{l(l+1)}{r^2} + (\alpha_1\,\alpha_2)^2 + \alpha_2^2\left(\frac{A}{r^2} - \frac{B}{r}\right)\right]R(r) = 0, \tag{3}$$

where

$$\alpha_1 = \sqrt{\mu - E},$$
$$\alpha_2 = \sqrt{\mu + E},$$
$$\beta = \sqrt{(1+2\,l)^2 + 4\,A\,{\alpha_2}^2}. \qquad (4)$$

To solve Eq.(3) we first study the asymptotic behaviour of $R(r)$ for small r and large r. It is easy to see that for large r, $R(r) \to \mathrm{e}^{-\alpha_1\,\alpha_2\,r}$, and $R(r)$ becomes zero when $r \to \infty$. On the other hand, for small r, the solution of Eq.(3), which satisfies the necessary condition of finiteness, is $R(r) \to r^{(\beta-1)/2}$. The above analysis suggests that if we let

$$R(r) = r^{(\beta-1)/2}\mathrm{e}^{-\alpha_1\,\alpha_2\,r}\,u(r), \qquad (5)$$

then we can obtain the equation of $u(r)$ as

$$r\,u''(r) + (1+\beta-2\,\alpha_1\,\alpha_2\,r)\,u'(r) - \left[(1+\beta)\,\alpha_1\,\alpha_2 - {\alpha_2}^2\,B\right]\,u(r) = 0. \qquad (6)$$

Now letting

$$\rho(r) = 2\,\alpha_1\,\alpha_2\,r, \qquad (7)$$

we obtain

$$\rho\,u''(\rho) + (1+\beta-\rho)\,u'(\rho) - \frac{1}{2}\left(1+\beta-\frac{\alpha_2}{\alpha_1}\,B\right)\,u(\rho) = 0. \qquad (8)$$

This is a confluent hypergeometric equation,[11] its solution is

$$u\,(\rho) = \mathrm{F}\left[\frac{1}{2}\left(1+\beta-\frac{\alpha_2}{\alpha_1}\,B\right), 1+\beta, \rho\right], \qquad (9)$$

where F represents the confluent hypergeometric function $\mathrm{F}[\alpha,\gamma,z]$.[11] For bound states, the confluent hypergeometric function $\mathrm{F}[\alpha,\gamma,z]$ will become a polynomial, which demands

$$\frac{1}{2}\left(1+\beta-\frac{\alpha_2}{\alpha_1}\,B\right) = -n \qquad (n=0,1,2,\cdots). \qquad (10)$$

Combining Eqs.(10) and (4) yields the energy equation

$$\left(1+2\,n+\sqrt{(2\,l+1)^2+4\,A\,(E+\mu)}\right) \times \sqrt{\mu-E} - B\,\sqrt{\mu+E} = 0. \qquad (11)$$

Although we can exactly solve Eq.(11) for E, the expression of E is too complicated to see its meaning. So we rewrite Eq.(11) as

$$-B\,\sqrt{2\,\mu-{\alpha_1}^2} + \alpha_1\left(1+2\,n+\sqrt{(2\,l+1)^2+4\,A\,(2\,\mu-{\alpha_1}^2)}\right) = 0 \qquad (12)$$

and expand it as a power series of α_1

$$-B\,\sqrt{2\,\mu}+\left(1+2\,n+\sqrt{(2\,l+1)^2+8\,\mu\,A}\right)\alpha_1 + \frac{B}{2\,\sqrt{2\,\mu}}\,\alpha_1^2 - \frac{2\,A}{\sqrt{(2\,l+1)^2+8\,\mu\,A}}\,\alpha_1^3 + \frac{B}{16\,\sqrt{2}\,\mu^{3/2}}\,\alpha_1^4 + \cdots = 0. \qquad (13)$$

If we only take the terms of α_1 as an approximation, and solve the energy equation, we have

$$E' = E-\mu = -\alpha_1^2 = -\frac{2\,\mu\,B^2}{\left(1+2\,n+\sqrt{(2\,l\,+1)^2+8\,\mu\,A}\right)^2}. \qquad (14)$$

In the above equation, E' is just the non-relativistic energy.[7] Finally, using the relation of the confluent hypergeometric function with Laguerre polynomial and the normalization condition of Laguerre polynomial,[11] we obtain the normalized radial wavefunction

$$R(r) = C\,r^{\frac{\beta-1}{2}}\mathrm{e}^{-\alpha_1\,\alpha_2\,r}\,\mathrm{F}\left[-n, 1+\beta, 2\,\alpha_1\,\alpha_2\,r\right], \qquad (15)$$

where the normalization constant is

$$C = \frac{(2\,\alpha_1\,\alpha_2)^{\frac{\beta}{2}+1}}{\Gamma(1+\beta)}\sqrt{\frac{\Gamma(1+n+\beta)}{(1+2\,n+\beta)\,\Gamma(1+n)}}. \qquad (16)$$

3. Bound-state solution of the Dirac equation with scalar and vector potentials equal to each other

The Dirac equation with scalar potential $s(r)$ and vector potential $v(r)$ is ($\hbar = c = 1$)

$$\{\boldsymbol{\alpha}\cdot\boldsymbol{P} + \beta[\mu + s(r)]\}\psi = [E - v(r)]\psi. \qquad (17)$$

In relativistic quantum mechanics, the complete set of the conservative quantities of a particle in a central field can be taken as (H, K, J^2, J_z), the eigenfunctions of which are[8]

$$\psi = \frac{1}{r}\begin{bmatrix} F(r)\phi^A_{jm_j} \\ \mathrm{i}G(r)\phi^B_{jm_j} \end{bmatrix} \qquad (K = j+1/2), \qquad (18)$$

$$\psi = \frac{1}{r}\begin{bmatrix} F(r)\phi^B_{jm_j} \\ \mathrm{i}G(r)\phi^A_{jm_j} \end{bmatrix} \quad (K=-(j+1/2)), \quad (19)$$

where

$$\phi^A_{jm_j} = \frac{1}{\sqrt{2\,l+1}}\begin{bmatrix} \sqrt{l+m+1}\,\mathrm{Y}_{l,m} \\ \sqrt{l-m}\,\mathrm{Y}_{l,m+1} \end{bmatrix},$$

$$\phi^B_{jm_j} = \frac{1}{\sqrt{2\,l+3}}\begin{bmatrix} -\sqrt{l-m+1}\,\mathrm{Y}_{l+1,m} \\ \sqrt{l+m+1}\,\mathrm{Y}_{l+1,m+1} \end{bmatrix}. \quad (20)$$

Substituting Eq.(18) or Eq.(19) into Eq.(17), we obtain the radial part of Dirac equation as

$$\begin{aligned} \frac{\mathrm{d}F}{\mathrm{d}r} - \frac{K}{r}F &= [\mu + E + s(r) - v(r)]\,G, \\ \frac{\mathrm{d}G}{\mathrm{d}r} + \frac{K}{r}G &= [\mu - E + s(r) + v(r)]\,F. \end{aligned} \quad (21)$$

Taking $s(r)=v(r)=\frac{1}{2}\left(\frac{A}{r^2}-\frac{B}{r}\right)$ in Eq.(21) leads to the following equations:

$$\begin{aligned} \frac{\mathrm{d}F}{\mathrm{d}r} - \frac{K}{r}F &= (\mu + E)\,G, \\ \frac{\mathrm{d}G}{\mathrm{d}r} + \frac{K}{r}G &= \left(\mu - E + \frac{A}{r^2} - \frac{B}{r}\right)F. \end{aligned} \quad (22)$$

Eliminating G from Eq.(22), we obtain

$$\begin{aligned} &F''(r) - \frac{K\,(K\,-\,1)}{r^2}F(r) \\ &-\alpha_2^2\left({\alpha_1}^2 + \frac{A}{r^2} - \frac{B}{r}\right)F(r) = 0, \end{aligned} \quad (23)$$

where α_1 and α_2 are the same as in Eq.(4). Using the same procedure for solving Eq.(3) and letting

$$\begin{aligned} F(r) &= \mathrm{e}^{-\rho/2}\,\rho^{(\beta+1)/2}\,f(\rho), \\ \rho &= 2\,\alpha_1\,\alpha_2\,r, \\ \beta &= \sqrt{(2\,K-1)^2 + 4\,A\,\alpha_2^2}, \end{aligned} \quad (24)$$

we obtain a confluent hypergeometric equation again from Eq.(23)

$$\begin{aligned} &\rho\,f''(\rho) + (1+\beta-\rho)\;f'(\rho) \\ &-\left(\frac{1+\beta}{2} - \frac{\alpha_2\,B}{2\,\alpha_1}\right)f(\rho) = 0. \end{aligned} \quad (25)$$

The solution of Eq.(25) is the confluent hypergeometric function

$$f(\rho) = \mathrm{F}\left[\frac{1+\beta}{2} - \frac{\alpha_2\,B}{2\,\alpha_1}, 1+\beta, \rho\right]. \quad (26)$$

For bound states, the confluent hypergeometric function $\mathrm{F}[\alpha,\gamma,z]$ must be turned to a polynomial, i.e.

$$\frac{1+\beta}{2} - \frac{\alpha_2\,B}{2\,\alpha_1} = -n \quad (n=0,1,2,\cdots). \quad (27)$$

This equation together with Eqs.(4) and (24) determines the energy equation

$$\begin{aligned} &\left(1+2\,n+\sqrt{(2\,K-1)^2+4\,A\;(E+\mu)}\right) \\ &\times\sqrt{\mu-E} - B\,\sqrt{\mu+E} = 0. \end{aligned} \quad (28)$$

Although Eq.(28) has an analytic solution for E, yet as in the case of previous section, the expression of E is too complicated to be understood, so we expand Eq.(28) as a series of α_1, and only take the first two terms, then we have

$$\begin{aligned} E' =& E-\mu = -\alpha_1^2 \\ =& -\frac{2\,\mu\,B^2}{\left(1+2\,n+\sqrt{(2\,K\,-1)^2+8\,\mu\,A}\right)^2}. \end{aligned} \quad (29)$$

Here E' is just the non-relativistic energy.[7]

Now, we can use n to express $F(r)$, and substitute Eqs.(24) and (26) into the first equation of Eq.(22) to gain $G(r)$. According to the normalization condition

$$\int_0^\infty \psi^\dagger\,\psi\,\mathrm{d}r = \int_0^\infty \left(|F(r)|^2 + |G(r)|^2\right)\mathrm{d}r = 1, \quad (30)$$

and by carrying out very tedious calculations, we finally obtain the normalized $F(r)$ and $G(r)$

$$F(r) = C\mathrm{e}^{-\alpha_1\,\alpha_2\,r}\,r^{(\beta+1)/2}\,\mathrm{F}\left[-n, 1+\beta, 2\,\alpha_1\,\alpha_2\,r\right], \quad (31)$$

$$\begin{aligned} G(r) =& -C\,(2\,\alpha_1\,\alpha_2^2)^{-1}\mathrm{e}^{-\alpha_1\,\alpha_2 r}r^{(\beta-1)/2} \\ &\times\{2\,n\,\alpha_1\,\mathrm{F}\left[1-n, 1+\beta, 2\,\alpha_1\,\alpha_2\,r\right] \\ &+(2\,\alpha_1\,K - B\,\alpha_2 + 2\,\alpha_1^2\,\alpha_2\,r) \\ &\times\mathrm{F}\left[-n, 1+\beta, 2\,\alpha_1\,\alpha_2\,r\right]\}, \end{aligned} \quad (32)$$

where the normalization constant is

$$C = \frac{\alpha_2\,(2\,\alpha_1\alpha_2)^{1+\beta/2}\,\sqrt{\Gamma(1+n+\beta)}}{\Gamma(\beta)\,\sqrt{\beta\,n!(A_1\,\alpha_1^2 - A_2\,\alpha_1\,\alpha_2 + A_3\,\alpha_2^2)}}, \quad (33)$$

and

$$\begin{aligned} A_1 =& 4\,(K+n)^2 + \beta\,(1+4\,K+6\,n+\beta), \\ A_2 =& 2\,B\;[2\,(K+n)+\beta], \\ A_3 =& B^2 + \beta\,(1+2n+\beta). \end{aligned} \quad (34)$$

Substituting $F(r)$ and $G(r)$ into Eqs.(18) and (19) yields the spinor wavefunction of Dirac equation.

4. Discussion

For $A = 0$ in Eq.(2), the potential we used becomes Coulomb potential. Letting $A = 0$ in Eqs.(11) and (28) and solving the corresponding energy equations, we obtain respectively

$$E = \mu \left(1 - \frac{2\,B^2}{B^2 + 4\,(1 + l + n)^2} \right), \qquad (35)$$

$$E = \mu \left(1 - \frac{2\,B^2}{B^2 + 4\,(K + n)^2} \right). \qquad (36)$$

Equations (35) and (36) are different from the relativistic energy formulae of hydrogen atom usually given by Klein–Gordon equation or Dirac equation. To further reveal this difference, We expand Eqs.(35) and (36) as series of parameter B,

$$E = \mu - \frac{\mu\,B^2}{2\,(1 + l + n)^2} + \frac{\mu\,B^4}{8\,(1 + l + n)^4} + O(B)^6, \qquad (37)$$

$$E = \mu - \frac{\mu\,B^2}{2\,(K + n)^2} + \frac{\mu\,B^4}{8\,(K + n)^4} + O(B)^6. \qquad (38)$$

The first terms on the right-hand of Eqs.(37) and (38) are the rest energy of the particle, the second terms are just the non-relativistic energy, but the third terms are not the same as the corresponding terms in the series expansion of relativistic hydrogen atomic energy.[10,12] This difference comes natural, because one usually considers the total Coulomb potential composed only of the vector potential and the scalar potential as zero. But in this paper we consider both the vector potential and the scalar potential equal to half of the total potential separately. And this equal vector and scalar potential model can eliminate some higher powers of r and makes it easier to solve relativistic quantum mechanics equations for some complicated potentials; however, whether this model can give more exact result for a relativistic quantum mechanics system needs further study in theory and experiment.

References

[1] Hou C F, Sun X D, Zhou Z X and Li Y 1999 *Acta Phys. Sin.* **48** 385 (in Chinese)

[2] Hou C F and Zhou Z X 1999 *Acta Phys. Sin.* (Overseas Edition) **8** 561

[3] Chen G 2001 *Acta Phys. Sin.* **50** 1651 (in Chinese)

[4] Chen C Y *et al* 2003 *Acta Phys. Sin.* **52** 1579 (in Chinese)

[5] Qiang W C 2002 *Chin. Phys.* **11** 757

[6] Qiang W C 2003 *Chin. Phys.* **12** 136

[7] Landau L D and Lifshitz E M 1958 *Quantum Mechanics* (London: Pergamon) p128

[8] Zeng J Y 1990 *Quantum Mechanics* (Vol I) (Beijing: Science Press) (in Chinese) pp315–6

[9] Qian B C and Zeng J Y 1999 *The Choiceness and Anatomy for Problems of Quantum Mechanics* (Vol II) (Beijing: Science Press) (in Chinese) p 321

[10] Wu T Y and Pauchy Hwang W Y 1991 *Relativistic Quantum Mechanics and Quantum Fields* (Singapore: World Scientific) p189

[11] Wang Z X and Guo D R 2000 *Introduction to Special Function* (Beijing: Peking University Press) (in Chinese) p288,321

[12] Berestetsiĭ V B, Lifshitz E, Pitaevskiĭ M 1971 *Relativistic Quantum Theory* (Part 1) (New York: Pergamon) p112