Analytical approximations of scattering states to the l-wave solutions for the Schrödinger equation with the Eckart potential

2008 J. Phys. A: Math. Theor. 41 035302

(http://iopscience.iop.org/1751-8121/41/3/035302)

J. Phys. A: Math. Theor. **41** (2008) 035302 (6pp) doi:10.1088/1751-8113/41/3/035302

Analytical approximations of scattering states to the *l*-wave solutions for the Schrödinger equation with the Eckart potential

Chang-Yuan Chen, Dong-Sheng Sun and Fa-Lin Lu

Department of Physics, Yancheng Teachers College, Yancheng 224002, People's Republic of China

E-mail: yctcccy@163.net (Chen C Y)

Received 9 October 2007, in final form 16 November 2007
Published 4 January 2008
Online at stacks.iop.org/JPhysA/41/035302

Abstract
The scattering state solutions of the Schrödinger equation for the Eckart potential with the centrifugal term are obtained approximately. It is shown that the solutions can be expressed in terms of the generalized hypergeometric functions ${}_2F_1\,(a, b; c; z)$. The normalized radial wave functions of scattering states on the '$k/2\pi$ scale' and the calculation formula of phase shifts are also derived. Three special cases for $l = 0$, $\beta = 0$ and $r_0 \to \infty$ are also studied briefly.

PACS numbers: 03.65.Nk, 03.65.Db.

1. Introduction

It is known that the exact solutions of the wave equations (non-relativistic or relativistic) are very important since they contain all the necessary information regarding the quantum system under consideration. However, analytical solutions are possible only in a few simple cases such as the hydrogen atom, the harmonic oscillator and others [1, 2]. Most quantum systems could only be treated by approximation methods. A typical example is the rotating Morse potential by the Pekeris approximation [3, 4]. Recently, the study of exponential-type potentials has attracted much attention from many authors [5–15]. These potentials include the Hulthén potential [5–7], the Rosen–Manning potential [8–11] and the Eckart potential [12–15].

The Eckart potential introduced by him [16] has been widely applied in physics [17] and chemical physics [18, 19]. In spherical coordinates (r, θ, ϕ), this potential is defined by

$$V(r) = -\alpha \frac{e^{-r/r_0}}{1 - e^{-r/r_0}} + \beta \frac{e^{-r/r_0}}{(1 - e^{-r/r_0})^2}, \qquad \alpha, \beta > 0. \tag{1}$$

Here, the parameters α and β describe the depth of potential well, while the parameter r_0 is related to the range of the potential. When $\beta = 0$, the Eckart potential reduces to the Hulthén potential.

The purpose of the present paper is to study the characteristics of scattering states for the Eckart potential. The reasons we write this paper are as follows. On the one hand, we have not yet found the scattering states related to this potential reported in previous literature. On the other hand, the theoretical prediction of many properties of quantum systems require the knowledge of radial wavefunctions of scattering states and the phase shifts.

This paper is organized as follows. In section 2, we show how to derive the arbitrary l-state solutions of scattering states for the Schrödinger equation with the Eckart potential by the approximate method since it gives the necessary repulsive core due to angular momentum. The normalized radial wave functions of scattering states on the '$k/2\pi$ scale' and the calculation formula of phase shifts are presented. Section 3 is devoted to three special cases for $l = 0$, $\beta = 0$ and $r_0 \to \infty$. The concluding remarks are given in section 4.

2. Analytical approximations of scattering states

We start from the Schrödinger equation with natural units $\hbar = \mu = 1$.

$$-\tfrac{1}{2}\nabla^2\psi(r,\theta,\varphi) + V(r)\psi(r,\theta,\varphi) = E\psi(r,\theta,\varphi), \tag{2}$$

where the potential $V(r)$ is taken as the Eckart form in equation (1). By taking $\psi(r,\theta,\varphi) = r^{-1}u(r)Y_{lm}(\theta,\varphi)$ and separating variable equation (2), we can obtain the radial equation as

$$\frac{\mathrm{d}^2u(r)}{\mathrm{d}r^2} + \left[2E + \frac{2\alpha\,\mathrm{e}^{-r/r_0}}{1-\mathrm{e}^{-r/r_0}} - \frac{2\beta\,\mathrm{e}^{-r/r_0}}{(1-\mathrm{e}^{-r/r_0})^2} - \frac{l(l+1)}{r^2}\right]u(r) = 0. \tag{3}$$

For the scattering states, $E > 0$. The boundary conditions are

$$r \to 0, \quad u(r) \to r^{l+1}; \qquad r \to \infty, \quad u(r) \to 2\sin(kr - \pi l/2 + \delta_l), \tag{4}$$

where $k = \sqrt{2E}$ and δ_l is the phase shift of the l-wave. The radial wavefunctions of scattering states for satisfying this boundary conditions are normalized on the '$k/2\pi$ scale'[2, 20].

Equation (3) cannot be solved analytically for $l \neq 0$ due to the centrifugal term. Therefore, we must use an approximation for this centrifugal term similar to the bound states [5, 15]. Their calculations show that this approximation can give results in good agreement with the results of the other methods [21] for large r_0 values. It is noted that for large values of the parameter r_0, i.e., for small r/r_0 the following formula

$$\frac{1}{r^2} \approx \frac{\mathrm{e}^{-r/r_0}}{r_0^2(1-\mathrm{e}^{-r/r_0})^2} \tag{5}$$

is a good approximation to $1/r^2$. By taking this approximation into account, defining a new variable $z = 1 - \mathrm{e}^{-r/r_0}$ ($r \in [0,\infty)$, $z \in [0,1]$)and equation (3) lead to

$$\frac{\mathrm{d}^2u}{\mathrm{d}z^2} - \frac{1}{1-z}\frac{\mathrm{d}u}{\mathrm{d}z} + \left(\frac{k^2r_0^2}{(1-z)^2} + \frac{\alpha'}{z(1-z)} - \frac{l'(l'+1)}{z^2(1-z)}\right)u = 0. \tag{6}$$

Here,

$$\alpha' = 2\alpha r_0^2, \qquad l' = \tfrac{1}{2}\left[\sqrt{4l(l+1) + 8\beta r_0^2 + 1} - 1\right]. \tag{7}$$

Considering the boundary conditions of the scattering states, we take the wavefunction with the form

$$u(z) = z^{l'+1}(1-z)^{-\mathrm{i}kr_0}f(z). \tag{8}$$

Substituting this into equation (6) allows us to obtain the following second-order differential equation

$$z(1-z)\frac{\mathrm{d}^2 f(z)}{\mathrm{d}z^2} + [2(l'+1) - (2l'+3-2\mathrm{i}kr_0)z]\frac{\mathrm{d}f(z)}{\mathrm{d}z} + [\alpha' - (l'+1)^2 + 2\mathrm{i}kr_0(l'+1)]f(z) = 0, \tag{9}$$

which is called the hypergeometric differential equation [22, 23]. Thus, the analytical solution is the hypergeometric function

$$f(z) = {}_2F_1(a, b; c; z). \tag{10}$$

The parameters are

$$a = l' + 1 + \sqrt{\alpha' - k^2 r_0^2} - \mathrm{i}kr_0, \qquad b = l' + 1 - \sqrt{\alpha' - k^2 r_0^2} - \mathrm{i}kr_0, \qquad c = 2l' + 2. \tag{11}$$

Here the hypergeometric function ${}_2F_1(a, b; c; z)$ is a special case of the generalized hypergeometric function [22, 23]

$${}_pF_q(\alpha_1, \alpha_2, \ldots, \alpha_p; \beta_1, \beta_2, \ldots, \beta_q; z) = \sum_{k=0}^{\infty} \frac{(\alpha_1)_k(\alpha_2)_k \ldots (\alpha_p)_k}{k!(\beta_1)_k(\beta_2)_k \ldots (\beta_q)_k} z^k, \tag{12}$$

where the Pochhammer symbol is defined by $(x)_k = \Gamma(x+k)/\Gamma(x)$. Thus, the radial wavefunction of scattering states is

$$u(r) = N_{kl'}(1 - \mathrm{e}^{-r/r_0})^{l'+1}\,\mathrm{e}^{\mathrm{i}kr}\,{}_2F_1(a, b; c; 1 - \mathrm{e}^{-r/r_0}). \tag{13}$$

We now study the asymptotic form of the above expression for large *r*, and calculate the normalization constant of radial wavefunctions $N_{kl'}$ and phase shifts. From formula (11), we have

$$c - a - b = 2\mathrm{i}kr_0 = (a + b - c)^*, \tag{14a}$$

$$c - a = l' + 1 - \sqrt{\alpha' - k^2 r_0^2} + \mathrm{i}kr_0 = b^*, \tag{14b}$$

$$c - b = l' + 1 + \sqrt{\alpha' - k^2 r_0^2} + \mathrm{i}kr_0 = a^*. \tag{14c}$$

By using the transformation formulae for hypergeometric functions [22, 23]

$${}_2F_1(a, b; c; z) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\,{}_2F_1(a, b; a+b-c+1; 1-z) + (1-z)^{c-a-b}\frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)}\,{}_2F_1(c-a, c-b; c-a-b+1; 1-z), \tag{15}$$

and paying attention to ${}_2F_1(a, b; c; 0) = 1$, we have

$$\begin{aligned}{}_2F_1(a, b; c; 1 - \mathrm{e}^{-r/r_0}) &= \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\,{}_2F_1(a, b; a+b-c+1; \mathrm{e}^{-r/r_0}) \\ &\quad + (\mathrm{e}^{-r/r_0})^{c-a-b}\frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)}\,{}_2F_1(c-a, c-b; c-a-b+1; \mathrm{e}^{-r/r_0}) \\ &\xrightarrow[r\to\infty]{} \Gamma(c)\left[\frac{\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} + \mathrm{e}^{-2\mathrm{i}kr}\left(\frac{\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\right)^*\right].\end{aligned} \tag{16}$$

Letting

$$\frac{\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} = \left|\frac{\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\right| \mathrm{e}^{\mathrm{i}\delta}, \tag{17a}$$

then

$$\left(\frac{\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\right)^* = \left|\frac{\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\right| \mathrm{e}^{-\mathrm{i}\delta}, \tag{17b}$$

where δ is a real number. Formula (16) then becomes

$${}_2F_1(a,b;c;1-\mathrm{e}^{-r/r_0}) \xrightarrow[r\to\infty]{} \Gamma(c)\left|\frac{\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\right| \mathrm{e}^{-\mathrm{i}kr}[\mathrm{e}^{\mathrm{i}(kr+\delta)} + \mathrm{e}^{-\mathrm{i}(kr+\delta)}]. \tag{18}$$

Substituting equation (18) into equation (13) leads to

$$\begin{aligned} u(r) &\xrightarrow[r\to\infty]{} 2N_{kl'}\Gamma(c)\left|\frac{\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\right| \cos(kr+\delta) \\ &\xrightarrow[r\to\infty]{} 2N_{kl'}\Gamma(c)\left|\frac{\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\right| \sin[kr-\pi l/2 + (\pi(l+1)/2+\delta)]. \end{aligned} \tag{19}$$

Comparing equations (4) with (19), we have the phase shifts as

$$\begin{aligned} \delta_l &= \pi(l+1)/2 + \arg\Gamma(c-a-b) - \arg\Gamma(c-a) - \arg\Gamma(c-b) \\ &= \pi(l+1)/2 + \arg\Gamma(2\mathrm{i}kr_0) - \arg\Gamma\left(l'+1+\mathrm{i}kr_0 - \sqrt{\alpha' - k^2r_0^2}\right) \\ &\quad - \arg\Gamma\left(l'+1+\mathrm{i}kr_0 + \sqrt{\alpha' - k^2r_0^2}\right), \end{aligned} \tag{20}$$

and the normalization constant on the '$k/2\pi$ scale' as

$$\begin{aligned} N_{kl'} &= \frac{1}{\Gamma(c)}\left|\frac{\Gamma(c-a)\Gamma(c-b)}{\Gamma(c-a-b)}\right| \\ &= \frac{1}{\Gamma(2l'+2)}\left|\frac{\Gamma\left(l'+1+\mathrm{i}kr_0 - \sqrt{\alpha'-k^2r_0^2}\right)\Gamma\left(l'+1+\mathrm{i}kr_0 + \sqrt{\alpha'-k^2r_0^2}\right)}{\Gamma(2\mathrm{i}kr_0)}\right|. \end{aligned} \tag{21}$$

3. Discussion

After approximately solving the scattering states of the l-wave Schrödinger equation with the Eckart potential, we should make three remarks.

(1) When $l = 0$, the centrifugal term $\frac{l(l+1)}{r^2} = 0$, and the approximation centrifugal term $\frac{l(l+1)\,\mathrm{e}^{-r/r_0}}{r_0^2(1-\mathrm{e}^{-r/r_0})^2} = 0$. Thus letting $l = 0$ in equation (7), we have $l' = \left(\sqrt{8\beta r_0^2+1}-1\right)/2$. Equations (20) and (21) reduce to the exact phase shift formula and the normalization constant on the '$k/2\pi$ scale' for the scattering states of the s-wave Schrödinger equation with the Eckart potential, respectively.

(2) From formula (7), when $\beta = 0$, $l' = \frac{1}{2}\left[\sqrt{4l(l+1)+8\beta r_0^2+1}-1\right] = l$, the integer l is the usual angular momentum quantum number. Then the Eckart potential reduces to the Hulthén potential (see equation (1)). Equations (20) and (21) reduce to the phase shifts and the normalization constant on the '$k/2\pi$ scale' of the Hulthén potential, respectively, i.e.

$$\begin{aligned} \delta_l &= \pi(l+1)/2 + \arg\Gamma(2\mathrm{i}kr_0) - \arg\Gamma\left(l+1+\mathrm{i}kr_0 - \sqrt{\alpha'-k^2r_0^2}\right) \\ &\quad - \arg\Gamma\left(l+1+\mathrm{i}kr_0 + \sqrt{\alpha'-k^2r_0^2}\right), \end{aligned} \tag{22}$$

$$N_{kl} = \frac{1}{(2l+1)!}\left|\frac{\Gamma\left(l+1+\mathrm{i}kr_0-\sqrt{\alpha'-k^2r_0^2}\right)\Gamma\left(l+1+\mathrm{i}kr_0+\sqrt{\alpha'-k^2r_0^2}\right)}{\Gamma(2\mathrm{i}kr_0)}\right|. \tag{23}$$

The above expressions are the same as the approximate analytical solutions of the l-wave scattering state for the Schrödinger equation with the Hulthén potential [7].

(3) When $\beta = 0$, $\alpha = Ze^2/r_0$, $r/r_0 \to 0$, the Eckart potential reduces to the Coulomb potential, i.e.

$$V(r) = -\alpha\frac{\mathrm{e}^{-r/r_0}}{1-\mathrm{e}^{-r/r_0}} + \beta\frac{\mathrm{e}^{-r/r_0}}{(1-\mathrm{e}^{-r/r_0})^2} = -\frac{Ze^2}{r_0}\cdot\frac{\mathrm{e}^{-r/r_0}}{1-\mathrm{e}^{-r/r_0}} \xrightarrow[r/r_0\to 0]{} -\frac{Ze^2}{r}. \tag{24}$$

From formulae (7) and (11), we can obtain $l' = l$, $\alpha' = 2Ze^2r_0$ and

$$\begin{aligned}\lim_{\beta=0,r_0\gg 1} a &= \lim_{\beta=0,r_0\gg 1}\left(l'+1+\sqrt{\alpha'-k^2r_0^2}-\mathrm{i}kr_0\right)\\ &= \lim_{r_0\gg 1}\left(l+1+\sqrt{2Ze^2r_0-k^2r_0^2}-\mathrm{i}kr_0\right)\\ &= l+1-\mathrm{i}Z/ka_0,\end{aligned} \tag{25}$$

$$\begin{aligned}\lim_{\beta=0,r_0\gg 1} b &= \lim_{\beta=0,r_0\gg 1}\left(l'+1-\sqrt{\alpha'-k^2r_0^2}-\mathrm{i}kr_0\right)\\ &= \lim_{r_0\gg 1}\left(l+1-\sqrt{2Ze^2r_0-k^2r_0^2}-\mathrm{i}kr_0\right)\\ &= \lim_{r_0\gg 1}(-2\mathrm{i}kr_0)\to\infty,\end{aligned} \tag{26}$$

where $a_0 = \hbar^2/\mu e^2$ is the Bohr radius. Using the relation of the hypergeometric function with the confluent hypergeometric function [22, 23],

$$\lim_{b\to\infty} {}_2F_1(a, b; c; z/b) = {}_1F_1(a; c; z), \tag{27}$$

we can rewrite the radial wavefunction (13) as

$$u(r) = A_{kl}(kr)^{l+1}\,\mathrm{e}^{\mathrm{i}kr}\,{}_1F_1(l+1-\mathrm{i}Z/ka_0; 2l+2; -2\mathrm{i}kr). \tag{28}$$

The above expression is the same as the radial wavefunction for the scattering states of the Schrödinger equation with the Coulomb potential [2, 20]. Where the normalization constant as

$$A_{kl} = \frac{2^{l+1}\,|\Gamma(l+1-\mathrm{i}Z/a_0k)|\,\mathrm{e}^{\pi Z/2a_0k}}{(2l+1)!}. \tag{29}$$

Now, we will discuss degradation of phase shifts. Since

$$\begin{aligned}\lim_{\beta=0,r_0\gg 1}\arg(c-a) &= \lim_{r_0\gg 1}\arg\left(l+1-\sqrt{2Ze^2r_0-k^2r_0^2}+\mathrm{i}kr_0\right)\\ &= \arg(l+1+\mathrm{i}Z/ka_0),\end{aligned} \tag{30}$$

$$\begin{aligned}&\lim_{\beta=0,r_0\gg 1}[\arg\Gamma(c-a-b)-\arg\Gamma(c-b)]\\ &\quad= \lim_{r_0\gg 1}\left[\arg\Gamma(2\mathrm{i}kr_0)-\arg\Gamma\left(l+1+\sqrt{2Ze^2r_0-k^2r_0^2}+\mathrm{i}kr_0\right)\right]\\ &\quad= \lim_{r_0\gg 1}[\arg\Gamma(2\mathrm{i}kr_0)-\arg\Gamma(l+1+2\mathrm{i}kr_0)]\\ &\quad= \lim_{r_0\gg 1}[\arg\Gamma(2\mathrm{i}kr_0)-\arg[(l+2\mathrm{i}kr_0)(l-1+2\mathrm{i}kr_0)\cdots(2\mathrm{i}kr_0)\Gamma(2\mathrm{i}kr_0)]]\\ &\quad= -\pi(l+1)/2.\end{aligned} \tag{31}$$

So formula (20) reduces to

$$\lim_{\beta=0, r_0 \gg 1} \delta_l = \pi(l+1)/2 + \arg\Gamma(c-a-b) - \arg\Gamma(c-a) - \arg\Gamma(c-b)$$
$$= -\arg\Gamma(l+1+\mathrm{i}Z/ka_0)$$
$$= \arg\Gamma(l+1-\mathrm{i}Z/ka_0). \tag{32}$$

The above expression is the same as the phase shifts for the Schrödinger equation with the Coulomb potential [2, 20].

4. Conclusions

In this paper, we have discussed characteristics of l-wave scattering states for the Eckart potential. Analytical approximations of scattering states to the l-wave solutions are deduced. The normalized radial wavefunctions of scattering states on the '$k/2\pi$ scale' and the calculation formula of phase shifts are presented. When $\beta = 0$, the Eckart potential reduces to the Hulthén potential, and when $\beta = 0$, $\alpha = Ze^2/r_0$ and $r/r_0 \to 0$, the Eckart potential reduces to the Coulomb potential. The results in this paper can reduce to solutions of scattering states of the Schrödinger equation with the Hulthén potential and the Coulomb potential.

Acknowledgments

We thank the referees for their useful suggestions. This work is supported by the Natural Science Foundation of the Jiangsu Higher Education Institutions of China under grant no. 06KJB140123.

References

[1] Schiff L I 1955 *Quantum Mechanics* 3rd edn (New York: McGraw-Hill)
[2] Landau L D and Lifshitz E M 1977 *Quantum Mechanics, Non-Relativistic Theory* 3rd edn (Oxford: Pergamon)
[3] Pekeris C L 1934 *Phys. Rev.* **45** 98
[4] Bayrak O and Boztosun I 2006 *J. Phys. A: Math. Gen.* **39** 6955
Qiang W C and Dong S H 2007 *Phys. Lett.* A **363** 169
[5] Bayrak O, Kocak G and Boztosun I 2006 *J. Phys. A: Math. Gen.* **39** 11521
[6] Bayrak O and Boztosun I 2007 *Phys. Scr.* **76** 92
[7] Chen C Y, Lu F L and Sun D S 2007 *Acta Phys. Sin.* **56** 6204 (in Chinese)
[8] Diaf A, Chouchaoui A and Lombard R J 2005 *Ann. Phys.* **317** 354
[9] Dong S H and García-Ravelo J 2007 *Phys. Scr.* **75** 307
[10] Qiang W C and Dong S H 2007 *Phys. Lett.* A **368** 13
[11] Chen C Y, Lu F L and Sun D S 2007 *Phys. Scr.* **76** 428
[12] Olğar E, Koç R and Tütüncüler H 2006 *Chin. Phys. Lett.* **23** 539
[13] Zou X, Yi L Z and Jia C S 2005 *Phys. Lett.* A **346** 54
[14] Jia C S, Guo P and Peng X L 2006 *J. Phys. A* **39** 7737
[15] Dong S H, Qiang W C, Sun G H and Bezerra V B 2007 *J. Phys. A* **40** 10535
[16] Eckart C 1930 *Phys. Rev.* **35** 1303
[17] Cooper F, Khare A and Sukhatme U 1995 *Phys. Rep.* **251** 267
[18] Weiss J J 1964 *J. Chem. Phys.* **41** 1120
[19] Cimas A, Aschi M, Barrientos C, Rayón V M, Sordo J A and Largo A 2003 *Chem. Phys. Lett.* **374** 594
[20] Zeng J Y 2000 *Quantum Mechanics* vol II 3rd edn (Beijing: Science Press) (in Chinese)
[21] Lucha W and Schöberl F F 1999 *Int. J. Mod. Phys.* C **10** 607
[22] Wang Z X and Guo D R 1979 *An Introduction to Special Functions* (Beijing: Science Press) (in Chinese)
[23] Gradshteyn I S and Ryzhik I M 2000 *Tables of Integrals, Series, and Products* 6th edn (New York: Academic Press)