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

2007 J. Phys. A: Math. Theor. 40 10535

(http://iopscience.iop.org/1751-8121/40/34/010)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **40** (2007) 10535–10540 doi:10.1088/1751-8113/40/34/010

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

Shi-Hai Dong[1], Wen-Chao Qiang[2], Guo-Hua Sun[3] and V B Bezerra[4]

[1] Departamento de Física, Esc Sup de Física y Matemáticas, Instituto Politécnico Nacional, Edificio 9, Unidad Profesional Adolfo López Mateos, Mexico DF 07738, Mexico
[2] Faculty of Science, Xi'an University of Architecture and Technology, Xi'an, 710055, People's Republic of China
[3] Universidad del Tepeyac, Av. Callao 802, Mexico D F 07300, Mexico
[4] Departamento de Física, Universidade Federal da Paraíba, 58059-970, João Pessoa, PB, Brazil

E-mail: dongsh2@yahoo.com, qwcqj@pub.xaonline.com and valdir@fisica.ufpb.br

Received 4 March 2007, in final form 10 July 2007
Published 7 August 2007
Online at stacks.iop.org/JPhysA/40/10535

Abstract
The bound-state solutions of the Schrödinger equation with 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 intractable normalized wavefunctions are also derived. To show the accuracy of our results, we calculate the eigenvalues numerically for arbitrary quantum numbers n and l. It is found that the results are in good agreement with those obtained by other methods for short-range potential (large a). Two special cases for $l = 0$ and $\beta = 0$ are also studied briefly.

PACS numbers: 03.65.Ge, 34.20.Cf

1. Introduction

The exact solutions of the stationary Schrödinger equation play an important role in quantum mechanics since they contain all the necessary information regarding the quantum system under consideration. However, it is possible to obtain only a few class of analytic solutions which correspond to some simple cases such as the hydrogen atom, the harmonic oscillator and others [1, 2]. In general, quantum systems can be treated only by approximation methods. A typical example is the rotating Morse potential treated by the Pekeris approximation [3, 4]. Recently, with the interest of the exponential-type potentials such as the Hulthén potential [5, 6], the multiparameter exponential-type potentials [7–10] and the Rosen-Manning potential [11, 12], the Eckart-type potential [13–15] given by

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

has been considered. Here, the parameters α and β describe the depth of potential well, while the parameter a is related to the range of the potential. The Eckart potential introduced by him [16] has been widely applied in physics [17] and chemical physics [18, 19]. On the other hand, it is found that the Eckart potential and its PT-symmetric version are the special cases of the five-parameter exponential-type potential model [9, 10]. It is shown that this potential has a minimum value $V(r_0) = -\frac{(\alpha-\beta)^2}{4\beta}$ at $r_0 = a\ln\left[\frac{\alpha+\beta}{\alpha-\beta}\right]$ for $\alpha > \beta$. The second derivative which determines the force constants at $r = r_0$ is given by

$$\left.\frac{\mathrm{d}^2 V}{\mathrm{d}r^2}\right|_{r=r_0} = \frac{(\alpha^2-\beta^2)^2}{8a^2\beta^3}. \tag{2}$$

It should be mentioned that most contributions appearing in the literature are concerned with the s-wave case besides [5, 6].

The purpose of this work is two-fold. First, we attempt to study the arbitrary l-state solutions of the Schrödinger equation with such a potential by approximate method, which has been used in a similar way to study the arbitrary l-state solutions of the Schrödinger equation with the Hulthén potential [5, 6]. Undoubtedly, this study will provide a good reference to interpret theoretically the quantum system with the arbitrary l states for the short-range potential. Second, the so-obtained eigenvalues are also to compare with numerical simulations of the eigenvalues for the non-approximated problem.

This paper is organized as follows. In section 2 we show how to derive the arbitrary l-state solutions of the Schrödinger equation with the Eckart potential by approximate method since it gives the necessary repulsive core due to angular momentum. In section 3 the numerical calculations are given and the results are compared with those obtained by other method. Section 4 is devoted to two special cases for $l = 0$ and $\beta = 0$. The concluding remarks are given in section 5.

2. Method

The Schrödinger equation in natural units $\hbar = \mu = 1$ is given by

$$\left\{-\frac{1}{2}\left[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] + V(r) - E\right\}\psi(\mathbf{r}) = 0. \tag{3}$$

By taking $\psi(\mathbf{r}) = r^{-1}R(r)Y_{lm}(\theta,\phi)$ and considering potential (1), we obtain the following radial Schrödinger equation:

$$\frac{\mathrm{d}^2 R(r)}{\mathrm{d}r^2} + \left[2E - \frac{2\beta\,\mathrm{e}^{-r/a}}{(1-\mathrm{e}^{-r/a})^2} + \frac{2\alpha\,\mathrm{e}^{-r/a}}{1-\mathrm{e}^{-r/a}} - \frac{l(l+1)}{r^2}\right]R(r) = 0. \tag{4}$$

This equation cannot be solved analytically for $l \neq 0$ due to the centrifugal term. Therefore, we must use an approximation[5] for this centrifugal term similar to the one used by other authors [5, 6, 20]. It is noted that for large values of the parameter a, i.e., for small r/a the following formula

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

is a good approximation to $1/r^2$. By taking this approximation into account, defining

$$z = \mathrm{e}^{-r/a}, \qquad \lambda = \sqrt{-2Ea^2}, \tag{6}$$

[5] Such an approximation was first introduced by Greene and Aldrich in order to generate pseudo- Hulthén wavefunctions for $l \neq 0$ states [20]. Considering the fact that the Hulthén potential is only the special case of the Eckart potential, we attempt to use a similar approximation to the Eckart potential so that we are able to study the arbitrary l-state solutions of the Schrödinger equation with this potential.

and substituting these into equation (4), we obtain

$$z^2\frac{\mathrm{d}^2R(z)}{\mathrm{d}z^2}+z\frac{\mathrm{d}R(z)}{\mathrm{d}z}-\left[\frac{Bz}{(1-z)^2}-\frac{Az}{1-z}+\frac{l(l+1)z}{(1-z)^2}+\lambda^2\right]R(z)=0, \qquad (7)$$

where $A=2\alpha a^2$ and $B=2\beta a^2$.

It is shown from equation (6) that $z\to 0(r\to\infty)$ and $z\to 1(r\to 0)$. As a result, the boundary conditions of the wavefunctions $R(z)$ are taken as follows:

$$R(z)\Rightarrow\begin{cases}0, & \text{when}\quad z\to 1,\\ 0, & \text{when}\quad z\to 0,\end{cases} \qquad (8)$$

from which we may take the radial wavefunctions $R(z)$ of the form

$$R(z)=(1-z)^{1+\delta}z^{\lambda}F(z), \qquad (9)$$

where

$$\delta=\tfrac{1}{2}\left[-1+\sqrt{(1+2l)^2+4B}\,\right]. \qquad (10)$$

Substitution of equation (9) into equation (7) leads to the following hypergeometric equation [21]:

$$(1-z)z\frac{\mathrm{d}^2F(z)}{\mathrm{d}z^2}+[2\lambda+1-z(2\delta+2\lambda+3)]\frac{\mathrm{d}F(z)}{\mathrm{d}z}$$
$$+[A-B-l(l+1)-(\delta+1)(1+2\lambda)]F(z)=0, \qquad (11)$$

whose solutions are nothing but the hypergeometric functions [21]

$$F(z)={}_2F_1(a,b;c;z)=\sum_{k=0}^{\infty}\frac{(a)_k(b)_k}{(c)_k}\frac{z^k}{k!}, \qquad (12)$$

where the parameters a, b, c and the Pochhammer symbol $(x)_k$ are given by

$$a=1+\delta+\lambda-\sigma,\qquad b=1+\delta+\lambda+\sigma,$$
$$c=1+2\lambda,\qquad (x)_k=\frac{\Gamma(x+k)}{\Gamma(x)}, \qquad (13)$$

with

$$\sigma=\sqrt{\lambda^2+A-B-l(l+1)+\delta(\delta+1)}. \qquad (14)$$

From the properties of the hypergeometric functions, this series $F(z)$ given in equation (12) approaches infinity unless $a=1+\delta+\lambda-\sigma$ is a negative integer. Therefore the radial wavefunctions $R(z)$ will not be finite everywhere unless

$$a=1+\delta+\lambda-\sigma=-n,\qquad n=0,1,2,\ldots, \qquad (15)$$

from which we have

$$\lambda=-\frac{(n+1)^2-A+B+l(l+1)+(2n+1)\delta}{2(n+\delta+1)}. \qquad (16)$$

Substitution of this into equation (6) leads to the following energy eigenvalues:

$$E_{nl}=-\frac{1}{2a^2}\left[\frac{(n+1)^2-A+B+l(l+1)+(2n+1)\delta}{2(n+\delta+1)}\right]^2. \qquad (17)$$

Now, let us study the eigenfunctions of this system. By using relation (15), we can write down the radial wavefunctions as

$$R(z)=N(1-z)^{\delta+1}z^{\lambda}{}_2F_1[-n,n+2(\delta+\lambda+1),2\lambda+1,z], \qquad (18)$$

Table 1. Eigenvalues (17) as a function of β for 2p, 3p and 3d states in atomic units ($\hbar = \mu = 1$) and for $\alpha = 1/a$.

		$\beta = 0.00005$		$\beta = 0.0001$	
	States $1/a$	Present	Schröberl	Present	Schröberl
2p	0.025	−0.111 363	−0.106 4737	−0.108 086	−0.100 8358
	0.050	−0.100 968	−0.099 4162	−0.100 574	−0.097 8358
	0.075	−0.090 161	−0.089 1284	−0.089 988	−0.088 4183
	0.100	−0.079 897	−0.078 7809	−0.079 788	−0.078 3854
	0.150	−0.061 191	−0.059 2734	−0.061 131	−0.059 1059
	0.200	−0.044 962	−0.041 7989	−0.044 925	−0.041 7120
	0.250	−0.031 225	−0.026 5616	−0.031 200	−0.026 5124
	0.300	−0.019 983	−0.013 7615	−0.019 967	−0.013 7330
	0.350	−0.011 239	−0.003 7780	−0.011 229	−0.013 7330
3p	0.025	−0.043 284	−0.041 8400	−0.042 284	−0.040 1250
	0.050	−0.033 267	−0.032 7011	−0.033 135	−0.032 2482
	0.075	−0.024 332	−0.023 7464	−0.024 275	−0.023 5553
	0.100	−0.016 774	−0.015 9559	−0.016 742	−0.015 8588
	0.150	−0.005 856	−0.004 4376	−0.005 844	−0.004 4091
3d	0.025	−0.043 407	−0.042 4588	−0.042 757	−0.041 3642
	0.050	−0.033 274	−0.032 4736	−0.033 165	−0.032 1973
	0.075	−0.024 333	−0.022 9146	−0.024 281	−0.022 7991
	0.100	−0.016 775	−0.014 4257	−0.016 743	−0.014 3675
	0.150	−0.005 856	−0.001 3808	−0.005 844	−0.001 3650

where N is the normalized factor to be determined from the normalization condition $\int_0^\infty R(r)^2\,\mathrm{d}r = 1$. This can be further written as

$$aN^2 \int_0^1 (1-z)^{2(\delta+1)} z^{2\lambda-1} \{{}_2F_1[-n, n+2(\delta+\lambda+1), 2\lambda+1, z]\}^2\,\mathrm{d}z = 1, \tag{19}$$

from which we obtain

$$N = \frac{1}{\sqrt{t(n)}},$$
$$t(n) = an!\Gamma(2\delta+3)\Gamma(2\lambda+1)\sum_{q=0}^{n} \frac{(-1)^q (n+2(\delta+\lambda+1))_q}{(q+2\lambda)(n-q)!q!\Gamma(q+2\delta+2\lambda+3)} \times {}_3F_2(-n, q+2\lambda, n+2\delta+2\lambda+2; 2\lambda+1, q+2\delta+2\lambda+3; 1), \tag{20}$$

where the Pochhammer symbol $(a)_n$ is defined above, and we have used the following integral formula [21]:

$$\int_0^1 z^{\varrho-1} z^{\sigma-1} {}_2F_1(\alpha,\beta;\gamma;z)\,\mathrm{d}z = \frac{\Gamma(\varrho)\Gamma(\sigma)}{\Gamma(\varrho+\sigma)} {}_3F_2(\alpha,\beta,\varrho;\gamma,\varrho+\sigma;1). \tag{21}$$

3. Numerical results

To show the accuracy of our results, we calculate the energy eigenvalues for arbitrary quantum numbers n and l. The results calculated by equation (17) are compared with those obtained by a MATHEMATICA package programmed by Lucha and Schöberl [22] as shown in tables 1 and 2. It is found that the results obtained by two different methods are in good

Table 2. Eigenvalues (17) as a function of β for 4p, 4d, 4f, 5p, 5d, 5f, 5 g, 6p, 6d, 6f and 6 g states in atomic units ($\hbar = \mu = 1$) and for $\alpha = 1/a$.

		$\beta = 0.00005$		$\beta = 0.0001$	
States	$1/a$	Present	Schröberl	Present	Schröberl
4p	0.025	−0.019 7893	−0.019 1787	−0.019 3674	−0.018 4632
	0.050	−0.011 207	−0.010 8852	−0.011 1533	−0.010 7159
	0.075	−0.004 9826	−0.004 5636	−0.004 9637	−0.004 5059
	0.100	−0.001 2436	−0.000 7380	−0.001 2370	−0.000 7212
4d	0.025	−0.019 8398	−0.019 3753	−0.019 5625	−0.018 9216
	0.050	−0.011 2098	−0.010 5633	−0.011 1644	−0.010 4603
	0.075	−0.004 9830	−0.003 8001	−0.004 9654	−0.003 7658
4f	0.025	−0.019 8615	−0.019 3525	−0.019 6478	−0.019 0220
	0.050	−0.011 211	−0.009 9876	−0.011 1692	−0.009 9137
	0.075	−0.004 9832	−0.002 5321	−0.004 9661	−0.002 5081
5p	0.025	−0.009 3460	−0.009 0320	−0.009 1391	−0.008 6850
	0.050	−0.002 7955	−0.002 5853	−0.002 7747	−0.002 5231
5d	0.025	−0.009 3703	−0.009 0768	−0.009 2332	−0.008 8576
	0.050	−0.002 7966	−0.002 2752	−0.002 7788	−0.008 8576
5f	0.025	−0.009 3807	−0.008 9892	−0.009 2743	−0.008 8297
	0.050	−0.002 7970	−0.001 7570	−0.002 7805	−0.001 7307
5g	0.025	−0.009 3866	−0.008 8194	−0.009 2973	−0.008 6943
	0.050	−0.002 7973	−0.000 9957	−0.002 7815	−0.000 9755
6p	0.025	−0.004 1446	−0.003 9648	−0.004 0376	−0.003 7873
6d	0.025	−0.004 1570	−0.003 9447	−0.004 0857	−0.003 8327
6f	0.025	−0.004 1623	−0.003 8337	−0.004 1067	−0.003 7525
6g	0.025	−0.004 1653	−0.003 6554	−0.004 1184	−0.003 5919

agreement for short-range potential (large a). However, the differences between them will appear for small values of the parameter a. This means that equation (5) is not a good approximation for a centrifugal term when the potential parameter a becomes small. In addition, it should be mentioned that the reason why we take the values of the parameter β very small is to make the Eckart potential well possess the bound states ($E < 0$).

4. Discussions

In this section, we are going to study two special cases of our results. First, let us study the s-wave case ($l = 0$). It is shown from equations (10) and (17) that

$$E_{nl} = \frac{-[-A + B + l(1+l) + (1+n)^2 + (-1 + \sqrt{1+4B})(1/2+n)]^2}{2a^2(1 + \sqrt{1+4B} + 2n)^2}. \tag{22}$$

Second, it is known that the Eckart potential reduces to the Hulthén potential for $\beta = 0$. If so, we have from equation (17)

$$E_{nl} = -\frac{[A - (l+n+1)^2]^2}{8a^2(l+n+1)^2}. \tag{23}$$

Finally, if taking $\alpha = Ze^2\delta$ and $\delta = 1/a$, we are able to obtain

$$E_{nl} = -\frac{1}{2}\left[\frac{1}{n+l+1} - \frac{(n+l+1)}{2a}\right]^2, \qquad (Z = e = 1), \tag{24}$$

where Z, e can be identified with the atomic number and the electron charge, respectively. This result coincides with that of [5].

5. Concluding remarks

The arbitrary l-state solutions of the Schrödinger equation with the Eckart potential have been presented approximately by considering equation (5). It is found that the solutions can be expressed by the generalized hypergeometric functions ${}_2F_1(a, b; c; z)$. The intractable normalized wavefunctions are also derived. To show the accuracy of our results, we have calculated the eigenvalues numerically for arbitrary n and l. We find that the results are in good agreement with those obtained by other method for short-range potential (large a). We have also studied two special cases for $l = 0$ and $\beta = 0$ and found that this potential reduces to the Hulthén potential when $\beta = 0$.

Acknowledgments

We would like to thank the kind referees and adjudicator for the invaluable and positive suggestions which improved the manuscript greatly. This work is supported partly by 20062088-SIP-IPN, 20070914-SIP-IPN, COFAA-IPN, Mexico and partly by Natural Science Basic Research Plan in Shaanxi Province of China (program no. 2005A22), NSF of the Education Bureau of Shaanxi Province of China under grant O5jk238, CNPq and FAPESQ-PB/CNPq(PRONEX)-Brazil.

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] Qiang W C and Dong S H 2007 *Phys. Lett.* A **363** 169 and references therein
[5] Bayrak O, Kocak G and Boztosun I 2006 *J. Phys. A: Math. Gen.* **39** 11521
[6] Gönül B, Özer O, Cançelik Y and Koçak M 2000 *Phys. Lett.* A **275** 238
[7] Eğrifes H, Demirhan D and Büyükkiliç F 2000 *Phys. Lett.* A **275** 229
[8] Jia C S, Diao Y F, Min L, Yang Q B, Sun L T and Huang R Y 2004 *J. Phys. A: Math. Gen.* **37** 11275
[9] Jia C S, Li Y, Sun Y, Liu J Y and Sun L T 2003 *Phys. Lett.* A **311** 115
[10] Jia C S, Zeng X L and Sun L T 2002 *Phys. Lett.* A **294** 185
[11] Dong S H and García-Ravelo J 2007 *Phys. Scr.* **75** 307
[12] Diaf A, Chouchaoui A and Lombard R J 2005 *Ann. Phys.* **317** 354
[13] Olğar E, Koç R and Tütüncüler H 2006 *Chin. Phys. Lett.* **23** 539
[14] Zou X, Yi L Z and Jia C S 2005 *Phys. Lett.* A **346** 54
[15] Jia C S, Guo P and Peng X L 2006 *J. Phys. A: Math. Gen.* **39** 7737
[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] Greene R L and Aldrich C 1976 *Phys. Rev.* A **14** 2363
[21] Gradshteyn I S and Ryzhik I M 1994 *Tables of Integrals, Series, and Products* 5th edn (New York: Academic)
[22] Lucha W and Schöberl F F 1999 *Int. J. Mod. Phys.* C **10** 607