Chin. Phys. B Vol. 19, No. 9 (2010) 090314

Approximate solutions of Schrödinger equation for Eckart potential with centrifugal term*

F. Taşkin and G. Koçak†
Department of Physics, Erciyes University, 38039 *Kayseri, Turkey*

(Received 14 January 2010)

The approximate analytical solutions of the Schrödinger equation for the Eckart potential are presented for the arbitrary angular momentum by using a new approximation of the centrifugal term. The energy eigenvalues and the corresponding wavefunctions are obtained for different values of screening parameter. The numerical examples are presented and the results are in good agreement with the values in the literature. Three special cases, i.e., s-wave, $\xi = \lambda = 1$, and $\beta = 0$, are investigated.

Keywords: Schrödinger equation, Eckart potential, bound state
PACC: 0365G, 0365C

1. Introduction

The solution of the Schrödinger equation with physical potentials by using different methods has an outgoing debate since the exact solutions of the Schrödinger equation with any potential play an important role in quantum mechanics. However, only in a few simple systems there exist analytical solutions such as the hydrogen atom, the harmonic oscillator in 3D and some other types of potentials.[1,2] The exact solution of the Schrödinger equation for the most of the physical potentials demonstrate difficulties in the case where the use of the approximation methods becomes necessary. The Eckart potential[3] is one of the most important exponential-type potentials in the literature and it has been widely used in physics[4] and chemical physics.[5,6] The s-wave solutions of the Schrödinger equation with the Eckart potential has been solved in Refs. [7]–[9]. Also, Klein–Gordon and Dirac equations with scalar and vector Eckart potentials have been studied to obtain bound state solutions of the s-wave case ($\ell = 0$).[10−12] Recently, Dong *et al.*[7] have used an approximation of the centrifugal term to obtain for any ℓ-wave case the bound state solution of the Schrödinger equation for the Eckart potential. Using the same approximation, scattering state problem of the Eckart potential[9,13] and the Dirac equation with the pseudo-centrifugal term[14,15] have been examined. But this approximation is acceptable for large values of the screening parameter.[7,16] For the Hulthén potential, Jia *et al.*[17] proposed a new approximation scheme to deal with the centrifugal term so as to prevent discrepancy between small and high screening parameter region. Here, we introduce a new modified approximation to obtain better results than those in Ref. [7] for not only high screening parameter but also small screening parameter.

In this work, we study ℓ state solutions of the Schrödinger equation for the Eckart potential by using a new approximation of the centrifugal term to acquire the small values of the screening parameter. In Section 2, we obtain the approximate closed forms of the energy eigenvalues and the corresponding wavefunctions. In order to test our results we gave the numerical examples (Tables 1 and 2). In Section 3, the relationships between our results and some other studies are discussed. Our conclusive remarks are given in the last section.

2. Bound state solutions

The Schrödinger equation is given by

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right]\Psi_{n\ell m}(r,\theta,\phi) = E\Psi_{n\ell m}(r,\theta,\phi), \quad (1)$$

where $V(r)$, μ and E are the spherical symmetric potential, the reduced mass and the bound sate energy of the system, respectively. Defining $\Psi_{n\ell m}(r,\theta,\phi) = (1/r)U_{n\ell}(r)Y_{\ell m}(\theta,\phi)$ and substituting it into Eq. (1), we obtain the radial part of the Schrödinger equation as follows:

$$\frac{\mathrm{d}^2U_{n\ell}(r)}{\mathrm{d}r^2} + \frac{2\mu}{\hbar^2}\left[E - V_{\mathrm{eff}}\right]U_{n\ell}(r) = 0, \quad (2)$$

*Project supported by the Scientific and Technological Council of Turkey TUBITAK under the Integrated PhD Program fellowship.
†Corresponding author. E-mail: ftaskin@erciyes.edu.tr
© 2010 Chinese Physical Society and IOP Publishing Ltd

where n and ℓ are the radial quantum number and the orbit angular momentum quantum number, respectively. In Eq. (2) the effective potential is define as

$$V_{\rm eff}(r) = V(r) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}. \tag{3}$$

The Eckart potential[3,10,7] is given by

$$V(r) = -\alpha\frac{{\rm e}^{-r/a}}{1-{\rm e}^{-r/a}} + \beta\frac{{\rm e}^{-r/a}}{(1-{\rm e}^{-r/a})^2}, \tag{4}$$

where α and β are the depths of the potential well, and a is the range of the potential. The effective potential with Eckart potential becomes

$$V_{\rm eff}(r) = V(r) + V_\ell(r) = -\alpha\frac{{\rm e}^{-r/a}}{1-{\rm e}^{-r/a}} + \beta\frac{{\rm e}^{-r/a}}{(1-{\rm e}^{-r/a})^2} + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}. \tag{5}$$

Substituting Eq. (5) into Eq. (2), we obtain

$$\frac{{\rm d}^2U_{n\ell}(r)}{{\rm d}r^2} + \frac{2\mu}{\hbar^2}\left[E + \alpha\frac{{\rm e}^{-r/a}}{1-{\rm e}^{-r/a}} - \beta\frac{{\rm e}^{-r/a}}{(1-{\rm e}^{-r/a})^2} - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right]U_{n\ell}(r) = 0. \tag{6}$$

Equation (6) can be solved exactly in the s-wave case for this potential. To find the approximate solution for the radial Schrödinger equation with the Eckart potential, we have to use an approximation for the centrifugal term. Dong *et al.*[7] have used an approximation of the centrifugal term and found the effective potential to be

$$\widehat{V}_{\rm eff}(r) = -\alpha\frac{{\rm e}^{-r/a}}{1-{\rm e}^{-r/a}} + \beta\frac{{\rm e}^{-r/a}}{(1-{\rm e}^{-r/a})^2} + \frac{\ell(\ell+1)\hbar^2}{2\mu a^2}\frac{{\rm e}^{-r/a}}{\left(1-{\rm e}^{-r/a}\right)^2}. \tag{7}$$

This approximation is good for large values of the parameter a, but it fails in the short-range region parameter.[7,16] For the validity of the approximation for low-screening region, we take a new approximation into account for the centrifugal term as follows:

$$\widetilde{V}_{\rm eff}(r) = -\alpha\frac{{\rm e}^{-r/a}}{1-{\rm e}^{-r/a}} + \beta\frac{{\rm e}^{-r/a}}{(1-{\rm e}^{-r/a})^2} + \frac{\ell(\ell+1)\hbar^2}{2\mu a^2}\left(\frac{\xi\,{\rm e}^{-r/a}}{1-q\,{\rm e}^{-r/a}} + \frac{\lambda\,{\rm e}^{-2r/a}}{\left(1-{\rm e}^{-r/a}\right)^2}\right), \tag{8}$$

where ξ and λ are adjustable dimensionless parameters. In order to show that the approximation given by Eq. (8) is better than that given by Eq. (7), we plot the variations of the $V_{\rm eff}(r)$, $\widehat{V}_{\rm eff}(r)$ and $\widetilde{V}_{\rm eff}(r)$ with r/a. In Fig. 1, the approximation given by Eq. (8) is much closer to the $V_{\rm eff}(r)$ than that given by Eq. (7) for small values of parameter a.

Substituting Eq. (8) into Eq. (6), we obtain the following second order differential equation:

$$\frac{{\rm d}^2U_{n\ell}(r)}{{\rm d}r^2} + \frac{1}{a^2}\left[-\varepsilon_{n\ell}^2 + \Phi\frac{{\rm e}^{-r/a}}{1-{\rm e}^{-r/a}} - \Theta\frac{{\rm e}^{-r/a}}{(1-{\rm e}^{-r/a})^2} + \lambda\gamma\frac{1-2\,{\rm e}^{-r/a}}{(1-{\rm e}^{-r/a})^2}\right]U_{n\ell}(r) = 0, \tag{9}$$

where

$$\varepsilon_{n\ell} = \sqrt{\lambda\gamma - \frac{2\mu a^2 E}{\hbar^2}}, \qquad \Phi = \frac{2\mu a^2\alpha}{\hbar^2} - \xi\gamma, \qquad \Theta = \frac{2\mu a^2\beta}{\hbar^2}, \qquad \gamma = \ell(\ell+1). \tag{10}$$

Defining a new variable of the form $z = {\rm e}^{-r/a}$ and substituting it into Eq. (9), the differential equation is given by

$$z^2\frac{{\rm d}^2U_{n\ell}(z)}{{\rm d}z^2} + z\frac{{\rm d}U_{n\ell}(z)}{{\rm d}z} + \left[-\varepsilon_{n\ell}^2 + \frac{\Phi\ z}{1-z} - \frac{\Theta\ z}{(1-z)^2} + \frac{\lambda\gamma\ (1-2z)}{(1-z)^2}\right]U_{n\ell}(z) = 0. \tag{11}$$

The boundary condition of the wavefunction $U_{n\ell}(z)$ is $z \to 0 (r \to \infty)$ and $z \to 1 (r \to 0)$. Under this condition, we can choose reasonable physical wavefunction as follows:

$$U_{n\ell}(z) = (1-z)^\sigma z^\rho f_{n\ell}(z), \tag{12}$$

where

$$\sigma = \frac{1}{2}\left(1 + \sqrt{1 + 4\lambda\gamma + 4\Theta}\right), \qquad \rho = \sqrt{\varepsilon_{n\ell}^2 - \lambda\gamma}. \tag{13}$$

Substituting the wavefunction given by Eq. (12) into Eq. (11), we obtain

$$(1-z)z\frac{\mathrm{d}^2 f_{n\ell}(z)}{\mathrm{d}z^2} + [2\rho + 1 - (2\rho + 2\sigma + 1)\, z]\frac{\mathrm{d}f_{n\ell}(z)}{\mathrm{d}z} - \left[(\rho+\sigma)^2 - \varepsilon_{n\ell}^2 - \Phi\right] f_{n\ell}(z) = 0. \tag{14}$$

The solution of this equation is just the hypergeometric function

$$f_{n\ell}(z) = {}_2F_1\,(a, b, 1 + 2\rho; z) = \frac{\Gamma(1+2\rho)}{\Gamma(a)\Gamma(b)}\sum_{k=0}^{\infty}\frac{\Gamma(a+k)\Gamma(b+k)}{\Gamma(1+2\rho+k)}\frac{z^k}{k!}, \tag{15}$$

where

$$a = \rho + \sigma + \sqrt{\varepsilon_{n\ell}^2 + \Phi}, \qquad b = \rho + \sigma - \sqrt{\varepsilon_{n\ell}^2 + \Phi}. \tag{16}$$

From the consideration of the finiteness of the solutions, it is shown from Eq. (15) that the general quantum condition is given by

$$a = \rho + \sigma + \sqrt{\varepsilon_{n\ell}^2 + \Phi} = -n, \qquad n = 0, 1, 2, 3, \ldots . \tag{17}$$

Using Eqs. (10), (13), (16) and (17), we obtain

$$E_{n\ell} = -\frac{\hbar^2}{2\mu a^2}\left[\frac{\Phi + \lambda\gamma}{2(n+\sigma)} - \frac{n+\sigma}{2}\right]^2, \tag{18}$$

which gives us the explicit expression for the any-ℓ-state energy eigenvalues of the Schrödinger equation for the Eckart potential.

To test the accuracy of Eq. (18), we calculate the energy eigenvalues for the Eckart potential with any n and ℓ quantum numbers and different values of the screening parameter $1/a$. Our results are compared with the results of the Dong *et al.*[7] and the MATHEMATICA package programmed by Lucha and Schöberl.[18] The adjustable parameters are taken to be $\xi = 1.10$ and $\lambda = 0.98$. The results are calculated by using the same parameter values as those in Ref. [7], but the authors have presented wrong analytical results. As it can be seen from Tables 1 and 2, our results are in good agrement with the findings from the other methods for the large a values. For small a values, there are small differences between our results and the results obtained from MATHEMATICA package programmed by Lucha and Schöberl.[18] It means that the approximation given by Eq. (8) is good for both small and large values of screening parameter to calculate the energy eigenvalues for the Eckart potential.

The corresponding unnormalized wavefunctions are given as

$$U_{n\ell}(r) = N(1 - \mathrm{e}^{-r/a})^{\sigma}\,\mathrm{e}^{-\rho r/a}\,{}_2F_1\left(-n, n + 2(\sigma+\rho); 1 + 2\rho; \mathrm{e}^{-r/a}\right), \tag{19}$$

where N is the normalization constant.

Table 1. The energy eigenvalues of the Eckart potential as a function of screening parameter $1/a$ for 2p, 3p and 3d states in atomic units ($\hbar = \mu = 1$). The other parameters are $\alpha = 1/a$, $\lambda = 0.98$ and $\xi = 1.10$.

states	$1/a$	$\beta = 0.0001$			$\beta = 0.00005$		
		present	Dong *et al.*[7]	Schöberl[18]	present	Dong *et al.*[7]	Schöberl[18]
2p	0.025	0.1015944	0.100888	0.1008358	0.1073496	0.106526	0.1064737
	0.050	0.0982980	0.098050	0.0978358	0.0999045	0.099630	0.0994162
	0.075	0.0885875	0.088880	0.0884183	0.0893055	0.089590	0.0891284

Table 1 (*continued*)

states	$1/a$	$\beta = 0.0001$			$\beta = 0.00005$		
		present	Dong *et al.*[7]	Schöberl[18]	present	Dong *et al.*[7]	Schöberl[18]
	0.100	0.0784035	0.079205	0.0783854	0.0788015	0.079600	0.0787809
	0.150	0.0592870	0.060920	0.0591059	0.0594540	0.061095	0.0592734
	0.200	0.0423448	0.044828	0.0417120	0.0427308	0.044914	0.0417989
	0.250	0.0286908	0.031152	0.0265124	0.0287387	0.031196	0.0265611
	0.300	0.0174777	0.019938	0.0137330	0.0175051	0.019970	0.0137615
	0.350	0.0090235	0.011214	0.0137330	0.0090385	0.011236	0.0037780
3p	0.025	0.0403106	0.040178	0.0401250	0.0420572	0.041894	0.0418400
	0.050	0.0323958	0.032454	0.0322482	0.0328534	0.032905	0.0327011
	0.075	0.0237732	0.023998	0.0235553	0.0239652	0.024188	0.0237464
	0.100	0.0162724	0.016610	0.0158588	0.0163698	0.016706	0.0159559
	0.150	0.0054340	0.005825	0.0044091	0.0054640	0.005850	0.0044376
3d	0.025	0.0414790	0.041519	0.0413642	0.0425903	0.042616	0.0424588
	0.050	0.0321085	0.032811	0.0321973	0.0323839	0.033089	0.0324736
	0.075	0.0229644	0.024150	0.0227991	0.0230774	0.024264	0.0229146
	0.100	0.0152256	0.016688	0.0143675	0.0152813	0.016747	0.0144257
	0.150	0.0044524	0.005845	0.0013650	0.0044680	0.005880	0.0013808

Table 2. The energy eigenvalues of the Eckart potential as a function of screening parameter $1/a$ for 4p, 4d, 4f, 5p, 5d, 5f, 5g, 6p, 6d, 6f and 6g states in atomic units ($\hbar = \mu = 1$). The other parameters are $\alpha = 1/a$, $\lambda = 0.98$ and $\xi = 1.10$.

states	$1/a$	$\beta = 0.0001$			$\beta = 0.00005$		
		present	Dong *et al.*[7]	Schöberl[18]	present	Dong *et al.*[7]	Schöberl[18]
4p	0.025	0.0185468	0.018514	0.0184632	0.0192709	0.019230	0.0191787
	0.050	0.0108554	0.010908	0.0107159	0.0110261	0.011078	0.0108852
	0.075	0.0047920	0.004874	0.0045059	0.0048493	0.004936	0.0045636
	0.100	0.0011400	0.001215	0.0007212	0.0011578	0.001229	0.0007380
4d	0.025	0.0189774	0.019076	0.0189216	0.0194354	0.019529	0.0193753
	0.050	0.0106863	0.011042	0.0104603	0.0107884	0.011146	0.0105633
	0.075	0.0045048	0.004924	0.0037658	0.0045386	0.004958	0.0038001
4f	0.025	0.0189461	0.019331	0.0190220	0.0192762	0.019661	0.0193525
	0.050	0.0102192	0.011102	0.0099137	0.0102901	0.011175	0.0099876
	0.075	0.0039915	0.004946	0.0025081	0.0040137	0.004972	0.0025321
5p	0.025	0.0087420	0.008735	0.0086850	0.0090910	0.009095	0.0090320
	0.050	0.0026616	0.002689	0.0025231	0.0027232	0.002744	0.0025853
5d	0.025	0.0089315	0.009000	0.0088576	0.0091505	0.009235	0.0090768
	0.050	0.0025859	0.002736	0.0088576	0.0026230	0.002771	0.0022752
5f	0.025	0.0088850	0.009130	0.0088297	0.0090440	0.009280	0.0089892
	0.050	0.0023989	0.002756	0.0017307	0.0024245	0.002785	0.0017570
5g	0.025	0.0087060	0.009205	0.0086943	0.0088280	0.009315	0.0088194
	0.050	0.0021281	0.002768	0.0009755	0.0021471	0.002792	0.0009957
6p	0.025	0.0038340	0.003831	0.0037873	0.0040128	0.004016	0.0039648
6d	0.025	0.0039244	0.003972	0.0038327	0.0040362	0.004090	0.0039447
6f	0.025	0.0038903	0.004034	0.0037525	0.0039716	0.004112	0.0038337
6g	0.025	0.0037866	0.004072	0.0035919	0.0038488	0.004134	0.0036554

3. Discussions

In this section, we study some special cases and the relationships between our results and those from the other studies in the literature.

First, let $\ell = 0$, we obtain the energy eigenvalues for the s-wave case,

$$E_{n0} = -\frac{\hbar^2}{2\mu a^2}\left[\frac{2\mu a^2\alpha/\hbar^2}{2n+1+\sqrt{1+8\mu a^2\beta/\hbar^2}} - \frac{2n+1+\sqrt{1+8\mu a^2\beta/\hbar^2}}{4}\right]^2, \tag{20}$$

which is the same as the result obtained in Ref. [7].

Second, when we set the adjustable dimensionless parameters to be $\xi = \lambda = 1$, the approximation given by Eq. (8) reduces to the approximation given by Eq. (7). In this case, the energy eigenvalues take the following forms ($\hbar = \mu = 1$):

$$E_{n\ell} = -\frac{1}{2a^2}\left[\frac{2a^2\alpha}{2n+1+\sqrt{1+4\ell(\ell+1)+8a^2\beta}} - \frac{2n+1+\sqrt{1+4\ell(\ell+1)+8a^2\beta}}{4}\right]^2, \tag{21}$$

which is the same as the result given by Eq. (17) in Ref. [7].

Third, choosing $\beta = 0$ in Eq. (4), the potential reduces to the Hulthén potential. In this case, Eq. (18) is given by

$$E_{n\ell} = -\frac{\hbar^2}{2\mu a^2}\left[\frac{\frac{2\mu a^2\alpha}{\hbar^2}+\ell(\ell+1)(\lambda-\xi)}{2n+1+\sqrt{1+4\lambda\ell(\ell+1)}} - \frac{2n+1+\sqrt{1+4\lambda\ell(\ell+1)}}{4}\right]^2, \tag{22}$$

which is the energy eigenvalues of the Schrödinger equation with the Hulthén potential. Substituting $\xi = \lambda = 1$ with $\delta = 1/a$ and $\alpha = Z\,\mathrm{e}^2\delta$ in atomic units into Eq. (22) yields obtain

$$E_{n\ell} = -\frac{1}{2}\left[\frac{1}{(n+\ell+1)} - \frac{(n+\ell+1)\delta}{2}\right]^2, \quad (Z=1), \tag{23}$$

which is the same as the result obtained in Ref. [16].

4. Conclusion

In this study, we investigate the solution of the Schrödinger equation for the Eckart potential by using the approximation given by Eq. (8) for the centrifugal term. We obtain the energy eigenvalues and the corresponding wavefunctions for several values of screening parameter for an arbitrary ℓ state. In Eq. (18), the case where $\ell = 0$, $\xi = \lambda = 1$ and $\beta = 0$ is briefly investigated. To show the accuracy of this approximation, we compare our results with the results of the Dong *et al.*[7] and the MATHEMATICA package programmed by Lucha and Schöberl.[18] Our results are in good agrement with those obtained by other methods for long-range screening parameter a. As can be seen in Fig. 1, this approximation works properly not only for small screening parameters but also for large screening parameters.

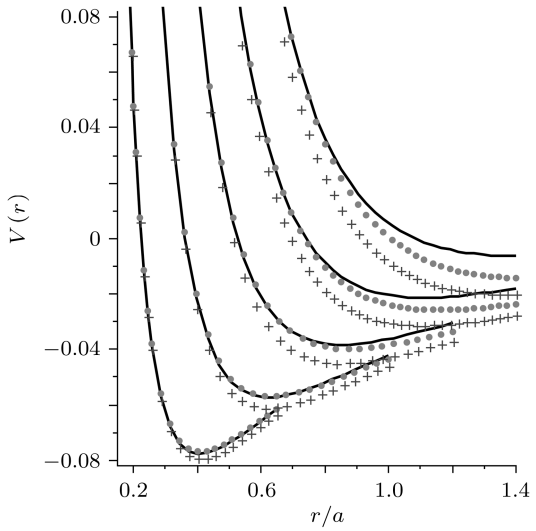


Fig. 1. The variations of the V_{eff} (solid line) and the approximate potentials $\widehat{V}_{\text{eff}}$ (cross) and $\widetilde{V}_{\text{eff}}$ (solid circle) with r/a for various values of the parameter. The $1/a$ changes from 0.10 to 0.30 in steps of 0.050. The other parameters are $\alpha = 1/a$, $\beta = 0.0001$, $\ell = 1$, $\lambda = 0.98$ and $\xi = 1.10$.

References

[1] Schiff L I 1955 *Quantum Mechanics* 3rd (New York: McGraw-Hill)

[2] Landau L D and Lifshitz E M 1977 *Quantum Mechanics, Non-Relativistic Theory* 3rd (Oxford: Pengamon)

[3] Eckart C 1930 *Phys. Rev.* **35** 1303

[4] Cooper F, Kahare A and Sukhatme U 1995 *Phys. Rept.* **251** 267

[5] Weiss J J 1964 *J. Chem. Phys.* **41** 1120

[6] Cimas A, Aschi M, Barrientos C, Rayòn V M, Sardo J A and Largo A 2003 *Chem. Phys. Lett.* **374** 594

[7] Dong S H, Qiang W C, Sun G H and Bezerra V B 2007 *J. Phys.* A: *Math. Theor.* **40** 10535

[8] Wei G F, Long C Y, Duan X Y and Dong S H 2008 *Phys. Scr.* **77** 035001

[9] Chen C Y, Sun D S and Lu F L 2008 *J. Phys.* A: *Math. Theor.* **41** 035302

[10] Zou X, Yi L Z and Jia C S 2005 *Phys. Lett.* A **346** 54

[11] Yi L Z, Diao Y F and Jia C S 2004 *Phys. Lett.* A **333** 212

[12] Jia C S, Guo P and Peng X L 2006 *J. Phys.* A: *Math. Gen.* **39** 7737

[13] Wei G F, Dong C Y, Sun G H and Bezerra V B 2008 *J. Phys.* A: *Math. Theor.* **40** 10535

[14] Zhang L H, Li X P and Jia C S 2008 *Phys. Lett.* A **372** 2201

[15] Soylu A, Bayrak O and Boztosun I 2008 *J. Phys.* A: *Math. Theor.* **41** 065308

[16] Bayrak O, Kocak G and Boztosun I 2006 *J. Phys.* A: *Math. Gen.* **39** 11521

[17] Jia C S, Liu J Y and Wang P Q 2008 *Phys. Lett.* A **372** 4779

[18] Lucha W and Schöberl F F 1999 *Int. J. Mod. Phys.* C **10** 607