Int J Theor Phys (2009) 48: 2692–2697
DOI 10.1007/s10773-009-0059-1

Approximate Solutions of the Schrödinger Equation for the Rosen-Morse Potential Including Centrifugal Term

F. Taşkın

Received: 18 December 2008 / Accepted: 4 June 2009 / Published online: 11 June 2009

Abstract Analytical solutions of the Schrödinger equation for the Rosen-Morse potential are presented for arbitrary orbital angular momentum quantum number by using an approximation for the centrifugal term. The energy eigenvalues and the corresponding wavefunctions are approximately obtained. Three special cases the s-wave, the Eckart potential and the PT-symmetric Rosen-Morse potential are also investigated.

Keywords Schrödinger equation · Rosen-Morse potential · Eckart potential · PT-symmetric Rosen-Morse potential · Bound state

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 the quantum mechanics. However, only in a few simple systems have analytical solutions such as the hydrogen atom, the harmonic oscillator in 3D and the others [1, 2]. Exact solutions of the Schrödinger equation for the most of the physical potentials demonstrate difficulties where the usage of an approximation method becomes a necessity. Recently, some authors have used an exponential type approximation for the centrifugal term to obtain the l-wave energy eigenvalues of the potentials, i.e., the Hulthén potential [3, 4], the Rosen-Manning potential [5–7], the Pöschl-Teller potential [8] and the Morse potential [9, 10].

The Rosen-Morse potential [11] is

$$V(r) = -V_1 \operatorname{sech}^2 \alpha r + V_2 \tanh \alpha r \tag{1}$$

where V_1 and V_2 are the depth of the potential and α is the range of the potential, respectively. This potential is useful for describing interatomic interaction of the linear molecules

F. Taşkın (✉)
Department of Physics, Erciyes University, 38039 Kayseri, Turkey
e-mail: ftaskin@erciyes.edu.tr

and helpful for discussing polyatomic vibration energies including the vibration states of NH_3 molecule [11]. The Rosen-Morse potential has a minimum value $V(r_0) = -\frac{4V_1^2+V_2^2}{4V_1}$ at $r_0 = -\text{arctanh}(\frac{V_2}{2V_1})$ for $|V_2| < 2V_1$. It is shown that the Rosen-Morse potential and its PT-symmetric version are the special cases of the five-parameter exponential-type potential model [12, 13]. Moreover, the exact energy spectrum of the trigonometric Rosen-Morse potential has been investigated by using supersymmetry and improved quantization rule methods [14, 15].

In this work, we have studied analytical solutions of the Schrödinger equation for the Rosen-Morse potential by using an approximation for centrifugal term. However, we have used an approximation [16] different from the previous works [3–10], $\frac{1}{r^2} \approx \alpha^2 \frac{e^{-\alpha r}}{(1-e^{-\alpha r})^2}$, which is not convenient for the Rosen-Morse type potential because one may not propose a reasonable physical wavefunction for the system. This paper is organized as follows. In Sect. 2, we have derived approximate l-wave solutions of the Schrödinger equation for the Rosen-Morse potential. Section 3 is devoted to three special cases the s-wave, the Eckart potential and the PT-symmetric Rosen-Morse potential. We have summarized our conclusion in Sect. 4.

2 Bound State Solutions

The Schrödinger equation of a particle with natural units ($\hbar = \mu = 1$) is given by

$$\left[-\frac{1}{2}\nabla^2 + V(r)\right]\Psi_{nlm}(r,\theta,\phi) = E\Psi_{nlm}(r,\theta,\phi) \tag{2}$$

where $V(r)$ and E are a spherical symmetric potential and the bound state energy of the system, respectively. Defining $\Psi_{nlm}(r,\theta,\phi) = r^{-1}U_{nl}(r)Y_{lm}(\theta,\phi)$ and substituting into (2), we obtain the radial part of the Schrödinger equation as follows

$$\frac{d^2U_{nl}(r)}{dr^2} + 2\left[E - V_{\mathit{eff}}\right]U_{nl}(r) = 0 \tag{3}$$

where n and l are the radial quantum number and the orbital angular momentum quantum number. Substituting effective potential $V_{\mathit{eff}}(r)$ with the Rosen-Morse potential into (3), we obtain

$$\frac{d^2U_{nl}(r)}{dr^2} + 2\left[E + V_1\text{sech}^2\alpha r - V_2\tanh\alpha r - \frac{l(l+1)}{2r^2}\right]U_{nl}(r) = 0. \tag{4}$$

Equation (4) can be solved exactly for the s-wave case ($l = 0$). To find an approximate solution for the radial Schrödinger equation with the Rosen-Morse potential, we have to use an approximation deal with the centrifugal term. Lu [16] has introduced an approximation for the centrifugal term for not too large l values and vibrations of the small amplitude close the minimum,

$$\frac{1}{r^2} \approx \frac{1}{r_0^2}\left[C_0 + C_1\frac{-e^{-2\alpha r}}{1+e^{-2\alpha r}} + C_2\left(\frac{-e^{-2\alpha r}}{1+e^{-2\alpha r}}\right)^2\right] \tag{5}$$

where

$$C_0 = 1 - \left(\frac{1+e^{-2\alpha r_0}}{2\alpha r_0}\right)^2 \left(\frac{8\alpha r_0}{1+e^{-2\alpha r_0}} - 3 - 2\alpha r_0\right), \tag{6}$$

$$C_1 = -2\left(1+e^{2\alpha r_0}\right)\left[3\left(\frac{1+e^{-2\alpha r_0}}{2\alpha r_0}\right) - (3+2\alpha r_0)\left(\frac{1+e^{-2\alpha r_0}}{2\alpha r_0}\right)\right], \tag{7}$$

$$C_2 = \left(1+e^{2\alpha r_0}\right)^2 \left(\frac{1+e^{-2\alpha r_0}}{2\alpha r_0}\right)^2 \left(3 + 2\alpha r_0 - \frac{4\alpha r_0}{1+e^{-2\alpha r_0}}\right). \tag{8}$$

Using the approximation given by (5), defining

$$z = -e^{-2\alpha r}, \qquad \lambda = \sqrt{\frac{\omega C_0}{4\alpha^2 r_0^2} + \frac{V_2}{2\alpha^2} - \frac{E}{2\alpha^2}}, \quad \omega = l(l+1), \tag{9}$$

and substituting (9) into (4), we obtain following second order differential equation

$$z^2 \frac{d^2 U_{nl}(z)}{dz^2} + z\frac{dU_{nl}(z)}{dz} - \left[\lambda^2 + \frac{2V_1}{\alpha^2}\frac{z}{(1-z)^2} + \left(\frac{V_2}{\alpha^2} + \frac{\omega C_1}{4\alpha^2 r_0^2}\right)\frac{z}{1-z} + \frac{\omega C_2}{4\alpha^2 r_0^2}\frac{z^2}{(1-z)^2}\right]U_{nl}(z) = 0. \tag{10}$$

The wavefunction $U_{nl}(z)$ has to satisfy the boundary conditions, i.e., $U_{nl}(0) = 0$ at $z \to 0$ ($r \to \infty$) and $U_{nl}(1) = 0$ at $z \to 1$ ($r \to 0$). As a result, we may take $U_{nl}(z)$ of the forms

$$U_{nl}(z) = (1-z)^{1+\delta} z^{\lambda} f_{nl}(z) \tag{11}$$

where

$$\delta = \frac{1}{2}\left(-1 + \sqrt{1 + \frac{8V_1}{\alpha^2} + \frac{\omega C_2}{\alpha^2 r_0^2}}\right). \tag{12}$$

Substituting the wavefunction given by (11) into (10), we obtain

$$z(1-z)\frac{d^2 f_{nl}(z)}{dz^2} + \left[2\beta + 1 - (2\delta + 2\lambda + 3)z\right]\frac{df_{nl}(z)}{dz} - \left[\frac{\omega C_1}{4\alpha^2 r_0^2} + \frac{2V_1 + V_2}{\alpha^2} + (1+\delta)(1+2\lambda)\right] f_{nl}(z) = 0. \tag{13}$$

The solution of (13) can be expressed in terms of the hypergeometric function, i.e.,

$$f_{nl}(z) = {}_2F_1(a, b; c; z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{k=0}^{\infty} \frac{\Gamma(a+k)\Gamma(b+k)}{\Gamma(c+k)} \frac{z^k}{k!} \tag{14}$$

where

$$a = 1 + \delta + \lambda - \chi, \qquad b = 1 + \delta + \lambda + \chi, \tag{15a}$$

$$c = 1 + 2\lambda, \qquad \chi = \sqrt{\lambda^2 - \frac{\omega C_1}{4\alpha^2 r_0^2} - \frac{2V_1 + V_2}{\alpha^2} + \delta(1+\delta)}. \tag{15b}$$

From the properties of the hypergeometric functions, the series given by (14) approaches infinity unless either a or b equals to a negative integer. Therefore, the wavefunction $U_{nl}(z)$ will not be finite everywhere unless

$$a = 1 + \delta + \lambda - \chi = -n, \quad n = 0, 1, 2, \ldots \tag{16}$$

from which we have

$$\lambda = -\frac{(n+1)^2 + \frac{2V_1+V_2}{\alpha^2} + \frac{\omega C_1}{4\alpha^2 r_0^2} + (2n+1)\delta}{2(n+\delta+1)}. \tag{17}$$

Using (9) into (17), we have an explicit expression for the energy eigenvalues of the Schrödinger equation with the Rosen-Morse potential

$$E_{nl} = \frac{\omega C_0}{2r_0^2} + V_2 - 2\alpha^2 \left[\frac{(n+1)^2 + \frac{2V_1+V_2}{\alpha^2} + \frac{\omega C_1}{4\alpha^2 r_0^2} + (2n+1)\delta}{2(n+\delta+1)} \right]^2. \tag{18}$$

Now, we can write the total radial wave function

$$U_{nl}(z) = N(1-z)^{1+\delta} z^{\lambda}\, {}_2F_1\left(-n, n + 2(1+\delta+\lambda); 1 + 2\lambda; z\right) \tag{19}$$

where N is the normalization constant. We are able to determine the normalization constant using the normalization condition ($\int_0^\infty U_{nl}^2(r)dr = 1$):

$$\frac{N^2}{2\alpha} \int_0^1 (1-z)^{2(1+\delta)} z^{2\lambda-1} \left[{}_2F_1\left(-n, n+2(1+\delta+\lambda); 1+2\lambda; z\right)\right]^2 dz = 1. \tag{20}$$

Using above equation and the following integral formula [17]

$$\int_0^1 (1-z)^{\mu-1} z^{\nu-1}\, {}_2F_1(\alpha, \beta; \gamma; az)dz = \frac{\Gamma(\mu)\Gamma(\nu)}{\Gamma(\mu+\nu)}\, {}_3F_2(\nu, \alpha, \beta; \mu+\nu, \gamma; a), \tag{21}$$

we have

$$N = \left[\frac{\Gamma(2\delta+3)\Gamma(2\lambda+1)}{2\alpha\Gamma(n)} \sum_{k=0}^{n} \frac{(-1)^k [n + 2(1+\delta+\lambda)]_k \Gamma(n+k)}{k!(k+2\lambda)\Gamma(k + 2(3/2+\delta+\lambda))} \right.$$
$$\left. \times\, {}_3F_2\left(2\lambda + k, -n, n + 2(1+\delta+\lambda); k + 2(3/2+\delta+\lambda), 1+2\lambda; 1\right) \right]^{-1/2} \tag{22}$$

where $(x)_k$ is the Pochhammer symbols and is given by

$$(x)_k = \frac{\Gamma(x+k)}{\Gamma(x)}. \tag{23}$$

3 Discussions

In this section, we investigate three special cases of (18). First, let us consider the s-wave case. Choosing $\beta = V_2/2\alpha^2$ and $\gamma = 2V_1/\alpha^2$, we obtain the energy eigenvalues of the system

$$E_{n0} = -\frac{8\alpha^2\beta}{2n+1+\sqrt{1+4\gamma}} + \frac{\alpha^2}{8}\left[2n+1+\sqrt{1+4\gamma}\right]^2 \quad (q=1) \tag{24}$$

which coincides with that of the reference [18]. In this case the number of discrete levels is finite since $E_{n0} > 0$ for $n < -4\sqrt{\beta} - (1+\sqrt{1+4\gamma})/2$.

Second, when we set $V_1 \to -V_1$, the potential reduces to the Eckart potential and the energy eigenvalues are given by

$$E_{nl} = \frac{\omega C_0}{2r_0^2} + V_2 - 2\alpha^2\left[\frac{\frac{\omega(C_2-C_1)}{4\alpha^2 r_0^2} - \frac{V_2}{\alpha^2}}{2(n+\delta_1+1)} - \frac{n+\delta_1+1}{2}\right]^2 \tag{25}$$

where $\delta_1 = \frac{1}{2}(-1+\sqrt{1-\frac{2V_1}{\alpha^2}+\frac{\omega C_2}{\alpha^2 r_0^2}})$.

Third, if we choose $V_2 \to -iV_2$, the potential becomes the PT-symmetric Rosen-Morse potential. For a potential $V(r)$, making the transformation of $r \to -r$ (or $r \to \xi - r$) and $i \to -i$, if we have the relation $V(-r) = V^*(r)$ (or $V(\xi - r) = V^*(r)$), the potential $V(r)$ is said to be PT-symmetric [12], where P denotes parity operator and T denotes time reversal. In this case, we obtain

$$E_{nl} = \frac{\omega C_0}{2r_0^2} + iV_2 - 2\alpha^2\left[\frac{(n+1)^2 + \frac{2V_1+iV_2}{\alpha^2} + \frac{\omega C_1}{4\alpha^2 r_0^2} + (2n+1)\delta}{2(n+\delta+1)}\right]^2 \tag{26}$$

where real $V_1 > 0$. If one set $l = 0$ in (26), the result coincides with the results of references [12, 13].

4 Conclusion

In this work, we have studied analytical approximate solutions of the Schrödinger equation for the Rosen-Morse potential including centrifugal potential term. To propose a reasonable physical wavefunction for the system, we have used the approximation given by (5) instead of the approximation used in references [3–10] for the centrifugal term. We have obtained approximate the energy eigenvalues and the corresponding wavefunctions depending on the α parameter. Three special cases the s-wave, the Eckart potential and the PT-symmetric Rosen-Morse potential are discussed. We have found that the s-wave energy eigenvalue of two special cases are in good agreement with the previous works [12, 13, 18].

Acknowledgement This work is partially supported by TUBITAK, the Scientific and Technological Council of Turkey.

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