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EXACT SOLUTIONS OF THE SCHRÖDINGER EQUATION FOR GENERALIZED HYPERBOLIC MOLECULAR POTENTIALS

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Abstract

In this paper, Schrödinger equations for generalized Rosen-Morse, generalized modified Rosen-Morse and generalized hyperbolic Kratzer-like potentials are solved. The energy eigenvalues and eigenfunctions of the bound states for the Schrödinger equation with these generalized potentials are derived by using the Nikiforov-Uvarov method. It is interesting to mention that the energy eigenvalues of the generalized Rosen-Morse potential depend on the deformation parameters of the generalized hyperbolic functions while the other two potentials are independent of these parameters. We conclude the paper with some comments and possible future work.

1. Introduction

It is well known that the study of exactly solvable problems has attracted much attention since the early development of quantum mechanics. For example, solutions of the Schrödinger equation for a hydrogen atom and a harmonic oscillator in 3D

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[17, 26]. Generally speaking, there are a few major methods to study solutions of quantum systems. The first is the so called traditional method which solves the generating second-order differential equation of quantum systems [15]. This can be realized by transforming the Schrödinger equation to some well-known ordinary differential equations, whose solutions are the special functions [18]. Also, studying the Hamiltonian of quantum systems is related with the method of the supersymmetric (SUSY) [6], and further closely with the factorization method [7, 21].

Recently, much attention has been paid to the exactly solvable Schrödinger equation of hyperbolic and triangular molecular potentials. Morse potential has been extensively studied in the last decades [18, 27]. For instance, the Morse potential as an important molecular potential describes the interaction between two atoms and has attracted a great deal of interest for some decades [23]. On the other hand, there are no analytical solutions for rotating Morse potential but the solution can be obtained numerically or semiclassical by using various approximate methods. One of these approximations is the Pekeris approximation [14, 25]. It has been used to obtain the semiclassical solutions. A number of semiclassical and numerical solutions for rotating Morse potential are presented [1, 3-5, 8, 12, 13, 17, 22]. Also, this approximation leads to other methods which include the variational [13], SUSY [6, 22], the hypervirial perturbation [17], the shifted $1/N$ expansion (SE) and the modified shifted $1/N$ expansion (MSE) [1], the asymptotic iteration methods (AIM) [3] and the Nikiforov-Uvarov (NU) [24].

More recently, an improved quantization rule was presented [21] as a powerful tool in calculating the energy levels of some exactly solvable quantum systems. They studied the systems such as the finite square well, the harmonic oscillator, the hydrogen atom, the Morse potential and its generalization, the symmetric and asymmetric hyperbolic type Rosen-Morse potentials, the symmetric and asymmetric Eckart potentials, the first and second Pöschl-Teller potentials and the Hulthén potential. Moreover, the rotating Morse potential within the Pekeris approximation [25], the cases of the deformed harmonic oscillator, the Kratzer potential and pseudoharmonic oscillator are carried out by using this quantization rule [7].

In this paper, we present the generalized hyperbolic functions [11, 16, 19, 20, 26] and its aspects. Based on these generalized functions, we introduce the generalized Rosen-Morse, generalized modified Rosen-Morse and hyperbolic Kratzer-like potentials. First, we take an interest in describing the generalized hyperbolic functions as follows:

$$\sinh_{pq}\xi = \frac{pe^{\xi} - qe^{-\xi}}{2}, \quad \cosh_{pq}\xi = \frac{pe^{\xi} + qe^{-\xi}}{2},$$

$$\tanh_{pq}\xi = \frac{\sinh_{pq}\xi}{\cosh_{pq}\xi}, \quad \mathrm{sech}_{pq}\xi = \frac{1}{\cosh_{pq}\xi}, \quad \xi \in \mathbb{C}, \tag{1.1}$$

where $p, q > 0$ are deformation parameters. Further, they carry up the following relations:

$$\sinh_{pq}(-\xi) = -pq\sinh_{\frac{1}{p}\frac{1}{q}}\xi, \quad \cosh_{pq}(-\xi) = pq\cosh_{\frac{1}{p}\frac{1}{q}}\xi,$$

$$(\sinh_{pq}\xi)' = \cosh_{pq}\xi, \quad (\cosh_{pq}\xi)' = \sinh_{pq}\xi,$$

$$(\tanh_{pq}\xi)' = pq\,\mathrm{sech}^2_{pq}\xi, \quad (\mathrm{sech}_{pq}\xi)' = -\mathrm{sech}_{pq}\xi\tanh_{pq}\xi,$$

$$\cosh^2_{pq}\xi - \sinh^2_{pq}\xi = pq, \quad \tanh^2_{pq}\xi = 1 - pq\,\mathrm{sech}^2_{pq}\xi, \quad \xi \in \mathbb{C}. \tag{1.2}$$

In conformity with the previous definitions (1.1), we rewrite the original Rosen-Morse potential which gives good results for molecular interaction [23] in the form:

$$V_{pq}(x) = B_0\tanh_{pq}(\alpha x) - \frac{U_0}{\cosh^2_{pq}(\alpha x)}$$

$$= B_0\frac{p - qe^{-2\alpha x}}{p + qe^{-2\alpha x}} - 4U_0\frac{e^{-2\alpha x}}{(p + qe^{-2\alpha x})^2}, \tag{1.3}$$

where α, B_0 and U_0 are arbitrary constants. It is easy to show that the minimum value of this potential is $x_{\min} = -\frac{1}{2\alpha}\ln\left[\frac{p(2U_0 + B_0pq)}{q(2U_0 - B_0pq)}\right]$.

Analogously, the hyperbolic Kratzer potential [2] can be generalized and taken the form

$$V_{pq}(x) = \frac{v_1}{2}(1 - \coth_{pq}(\alpha x)) + \frac{v_2}{4}(\coth^2_{pq}(\alpha x) - 1)$$

$$= -v_1q\frac{e^{-2\alpha x}}{p - qe^{-2\alpha x}} + v_2pq\frac{e^{-2\alpha x}}{(p - qe^{-2\alpha x})^2}, \tag{1.4}$$

where v_1 and v_2 are also arbitrary constants, with the same-manner, the minimum value takes the form $x_{\min} = -\frac{1}{2\alpha}\ln\left[\frac{p(v_1 - v_2)}{q(v_1 + v_2)}\right]$.

However, the generalized modified Rosen-Morse potential is

$$V_{pq}(x) = \frac{v_1}{2}(1 + \tanh_{pq}(\alpha x)) + \frac{v_2}{4}(\tanh^2_{pq}(\alpha x) - 1)$$

$$= \frac{v_1 p}{p + qe^{-2\alpha x}} - \frac{v_2 pqe^{-2\alpha x}}{(p + qe^{-2\alpha x})^2}. \tag{1.5}$$

This potential has a minimum value at $x_{\min} = -\frac{1}{2\alpha}\ln\left[\frac{p(v_2 + v_1)}{q(v_2 - v_1)}\right]$.

The aim of this paper is to solve the Schrödinger equation when the potential takes the previous formulas. Thus, we turn our attention to describe the method which used to solve problems like this. This will be done in the following section.

This paper is organized as follows. In the following section, we review the NU method. The energy eigenvalues and eigenfunctions of the bound states for the Schrödinger equation with the above potentials are presented in Sections 3 and 4. A brief summary and discussion are given in the last section.

2. Nikiforov-Uvarov Method

The NU method is based on solving a second-order linear equation by reducing it to a generalized equation of hyperbolic type. It used to solve the Schrödinger, Dirac and Klien-Gordon wave equations for a certain kind of potential [24]. In this method, the second-order differential equation is

$$\psi''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0, \tag{2.1}$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials, at most of second degree, and $\tilde{\tau}(s)$ is a first-degree polynomial. In order to find a particular solution to equation (2.1), we consider that

$$\psi(s) = \phi(s)y(s). \tag{2.2}$$

According to this transformation, equation (2.1) is

$$\sigma(s)y'' + \tau(s)y' + \lambda y = 0, \tag{2.3}$$

where $\phi(s)$ is defined as a logarithmic derivative

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)}. \tag{2.4}$$

The other part $y(s)$ is the hypergeometric-type function whose polynomial solutions are given by Rodrigues relation

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n}[\sigma^n(s)\rho(s)], \tag{2.5}$$

where B_n is a normalizing constant and the weight function $\rho(s)$ must satisfy the condition

$$(\sigma\rho)' = \tau\rho. \tag{2.6}$$

The function $\pi(s)$ and the parameter λ required for this method are defined as follows:

$$\pi(s) = \frac{\sigma' - \tilde{\tau}}{2} \pm \sqrt{\left(\frac{\sigma' - \tilde{\tau}}{2}\right)^2 - \tilde{\sigma} + k\sigma}, \tag{2.7}$$

$$\lambda = k + \pi'. \tag{2.8}$$

On the other hand, in order to find the value of k, the expression under the square root must be the square of a polynomial. Thus, a new eigenvalue equation for second-order differential equation becomes

$$\lambda = \lambda_n = -n\tau' - \frac{n(n-1)}{2}\sigma'', \tag{2.9}$$

where

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s), \tag{2.10}$$

and its derivative is negative. By the comparison of equations (2.8) and (2.9), we obtain the energy eigenvalues.

3. The Generalized Rosen-Morse Potential

It is well known that one-dimensional Schrödinger equation takes the form:

$$E\psi(x) = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi(x). \tag{3.1}$$

Therefore, for the generalized potentials of the bound states $(E < 0)$, we have

$$\psi''_{pq}(x) + \frac{2m}{\hbar^2}[E - V_{pq}(x)]\psi_{pq}(x) = 0. \tag{3.2}$$

When we presume the potential $V_{pq}(x)$ in the form (1.3), we have

$$\psi''_{pq}(x) + \frac{2m}{\hbar^2}\left[E - B_0\frac{p - qe^{-2\alpha x}}{p + qe^{-2\alpha x}} + 4U_0\frac{e^{-2\alpha x}}{(p + qe^{-2\alpha x})^2}\right]\psi_{pq}(x) = 0. \tag{3.3}$$

The following transformation $e^{-2\alpha x} = -s$ and after some algebraic calculations, equation (3.3) reduces to

$$\psi''_{pq}(s) + \frac{p - qs}{s(p - qs)}\psi'_{pq}(s)$$

$$+ \frac{1}{[s(p - qs)]^2}[(\beta - \varepsilon)q^2s^2 + (2\varepsilon pq - \gamma)s - (\beta + \varepsilon)p^2]\psi_{pq}(s) = 0, \tag{3.4}$$

where $\beta = \frac{mB_0}{2\alpha^2\hbar^2} > 0$, $\varepsilon = -\frac{mE}{2\alpha^2\hbar^2} > 0$ and $\gamma = \frac{2mU_0}{\alpha^2\hbar^2} > 0$. This equation is correspondence to equation (2.1) with

$$\tilde{\tau}(s) = p - qs, \quad \sigma(s) = s(p - qs),$$

$$\tilde{\sigma}(s) = (\beta - \varepsilon)q^2s^2 + (2\varepsilon pq - \gamma)s - (\beta + \varepsilon)p^2. \tag{3.5}$$

According to the NU method, we have

$$\pi(s) = -\frac{qs}{2} \pm \frac{1}{2}\sqrt{(q^2 - 4(\beta - \varepsilon)q^2 - 4kq)s^2 - 4(2\varepsilon pq - \gamma - kp)s + 4(\beta + \varepsilon)p^2}. \tag{3.6}$$

The constant k can be determined from the condition that the function under the square root has a double zero. Therefore, it takes the form

$$k = -\frac{\gamma}{p} - 2\beta q \pm q\sqrt{\beta+\varepsilon}\sqrt{1+\frac{4\gamma}{pq}}. \tag{3.7}$$

Now, the function $\pi(s)$ has

$$\pi(s)$$

$$= -\frac{qs}{2} \mp \frac{1}{2}\begin{cases}\left(2q\sqrt{\beta+\varepsilon} - q\sqrt{1+\frac{4\gamma}{pq}}\right)s - 2p\sqrt{\beta+\varepsilon}, & k = -\frac{\gamma}{p} - 2\beta q + q\sqrt{\beta+\varepsilon}\sqrt{1+\frac{4\gamma}{pq}}, \\ \left(2q\sqrt{\beta+\varepsilon} + q\sqrt{1+\frac{4\gamma}{pq}}\right)s - 2p\sqrt{\beta+\varepsilon}, & k = -\frac{\gamma}{p} - 2\beta q - q\sqrt{\beta+\varepsilon}\sqrt{1+\frac{4\gamma}{pq}}.\end{cases} \tag{3.8}$$

The polynomial $\pi(s)$ is preferred such that the function $\tau(s)$ given by equation (2.9) will have a negative derivative, by a suitable choice of $\pi(s)$ the function $\tau(s)$ takes the formula

$$\tau_{pq}(s) = p(1 + 2\sqrt{\beta+\varepsilon}) - q\left[2(1+\sqrt{\beta+\varepsilon}) - \sqrt{1+\frac{4\gamma}{pq}}\right]s, \tag{3.9}$$

where $\tau'_{pq}(s) = -q\left[2(1+\sqrt{\beta+\varepsilon}) - \sqrt{1+\frac{4\gamma}{pq}}\right] < 0,$ which corresponds to

$$\pi(s) = -\frac{qs}{2} - \frac{1}{2}\left(2q\sqrt{\beta+\varepsilon} - q\sqrt{1+\frac{4\gamma}{pq}}\right)s - 2p\sqrt{\beta+\varepsilon},$$

$$k = -\frac{\gamma}{p} - 2\beta q + q\sqrt{\beta+\varepsilon}\sqrt{1+\frac{4\gamma}{pq}}. \tag{3.10}$$

In this case, $\phi(s)$ and λ are given by

$$\phi(s) = s^{\sqrt{\beta+\varepsilon}}(p - qs)^{\frac{\nu}{2}}, \tag{3.11}$$

$$\lambda = -\frac{\gamma}{p} - 2\beta q + q\sqrt{\beta+\varepsilon}\sqrt{1+\frac{4\gamma}{pq}} - \frac{q}{2} - \frac{q}{2}\left(2\sqrt{\beta+\varepsilon} - \sqrt{1+\frac{4\gamma}{pq}}\right), \tag{3.12}$$

where $\nu = 1 - \sqrt{1 + \frac{4\gamma}{pq}}$. The other part $y_{npq}(s)$ is given by (2.5),

$$y_{npq}(s) = B_n s^{-2\sqrt{\beta+\varepsilon}}(p - qs)^{-(\nu-1)} \frac{d^n}{ds^n}[s^{n+2\sqrt{\beta+\varepsilon}}(p - qs)^{n+(\nu-1)}], \qquad (3.13)$$

where $\rho(s) = s^{2\sqrt{\beta+\varepsilon}}(p - qs)^{\nu-1}$. Moreover, the energy eigenvalues are determined through the equation

$$\lambda + n\tau' + \frac{n(n-1)}{2}\sigma'' = 0,$$

which gives

$$E_{npq} = -\frac{2\alpha^2\hbar^2}{m}\varepsilon_{npq}, \qquad (3.14)$$

where

$$\varepsilon_{npq} = \frac{1}{16}\left[-(2n+1) + \sqrt{1 + \frac{4\gamma}{pq}}\right]^2 + \frac{4\beta^2}{\left[-(2n+1) + \sqrt{1 + \frac{4\gamma}{pq}}\right]^2}. \qquad (3.15)$$

From the condition $\varepsilon_{npq} > 0$, the discrete level is finite and determined by the inequality $n < -\sqrt{2\beta} - \frac{\nu}{2}$. In particular, the wave function $\psi_{npq}(x)$ of the corresponding potential is

$$\psi_{npq}(s) = s^{\mu}(p - qs)^{\frac{\nu}{2}} y_{npq}(s), \quad n = \left(0, 1, 2, ..., -\sqrt{2\beta} - \frac{\nu}{2} - 1\right), \qquad (3.16)$$

where $\mu = \sqrt{\beta + \varepsilon_{npq}}$. The considered system is characterized by describing the Rosen-Morse potential in a general case, where we assumed the presence of two deformed parameters p and q. Moreover, if $p = 1$, we have the results of [9], while the results of [24] are given when $p = q = 1$. Further, it is obvious that the wave function (3.16) depends on the deformation parameters p, q. In addition, the energy eigenvalues E_{npq} given by equation (3.14) with the condition $\varepsilon_{npq} > 0$ lead to

$pq < 4\gamma/[[2n + 1 + 2\sqrt{2\beta}]^2 - 1]$. Consequently, if we take the parameters α and β with the values as in [9], we have the same curves of [9] when we take $p = 1$ as shown in Figure 1(a). By simple calculations, we get $pq < 5.1$ for $n = 0$, $pq < 2.4$ for $n = 1$, $pq < 1.4$ for $n = 2$, etc., thus the curves in Figure 1 do not cut one another. Again in the same figure,

$$E_{n(pq)_{\max}} \cong -U_0/4 \quad \text{for} \quad (pq)_{\max} = 4\gamma/[[2n + 1 + 2\sqrt{2\beta}]^2 - 1].$$

Based on the previous calculations, we can generalize the Pöschl-Teller potential [10] by putting $B_0 = 0$ in (1.3). In this case, the energy eigenvalues are

$$E_{npq} = -\frac{\alpha^2\hbar^2}{8m}\left[-(2n+1) + \sqrt{1 + \frac{4\gamma}{pq}}\right]^2. \tag{3.17}$$

Furthermore, the eigenfunctions from the Rodrigues relation given by equation (2.5) are acquired in the form:

$$y_{npq}(s) = B_n s^{-2\sqrt{\varepsilon}}(p - qs)^{-(\nu-1)} \frac{d^n}{ds^n}[s^{n+2\sqrt{\varepsilon}}(p - qs)^{n+(\nu-1)}], \tag{3.18}$$

where $\nu = 1 - \sqrt{1 + \frac{4\gamma}{pq}}$. Finally, the unnormalized wave functions $\psi_{npq}(x)$ are identified as

$$\psi_{npq}(s) = s^{\sqrt{\varepsilon}}(p - qs)^{\frac{\nu}{2}} y_{npq}(s), \quad n = \left(0, 1, 2, \ldots, -\frac{\nu}{2} - 1\right), \tag{3.19}$$

with $\varepsilon = \varepsilon_{npq} = \frac{1}{16}\left[-(2n+1) + \sqrt{1 + \frac{4\gamma}{pq}}\right]^2$.

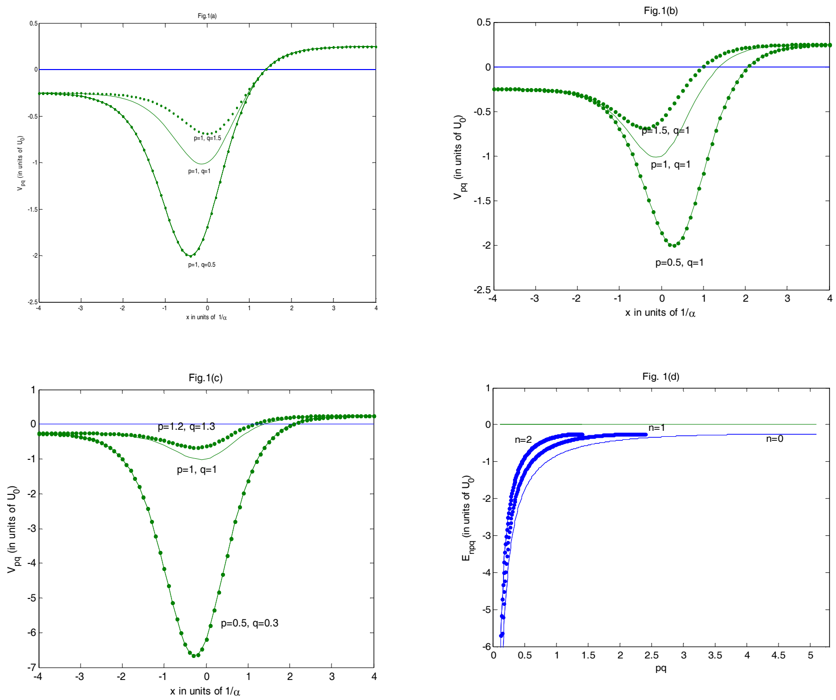

Figure 1. The generalized Rosen-Morse potential for different values of the deformation parameters p and q with $4\gamma = (8mU_0/\alpha^2\hbar^2) = 99$ and $B_0 = U_0/4$ (i.e., $\beta = \gamma/16$) is plotted in (a)-(c), (d) represents the variation of the energy levels characterized by the vibrational quantum number $[n]$ with respect to the deformation parameters p and q.

It is remarkable that when $p = 1$ and $q = 0.5, 1$ and 1.5, we have the same figure of [9] as shown in Figure 1(a). The effect of the parameter p when $q = 1$ is shown in Figure 1(b). We observe that as p increases, the minimum value of the potential decreases. On the other hand, the influence of the deformed parameters p and q is illustrated in Figure 1(c).

In what follows, we construct ourselves to another two systems, where we hypothesize the potentials are given by (1.4) and (1.5), respectively.

4. The Generalized Hyperbolic Kratzer and Modified Rosen-Morse Potentials

Now, we focus to solve the Schrödinger equation when the potential $V_{pq}(x)$ is given by (1.4). In this case, the Schrödinger equation takes the form

$$\psi''_{pq}(x)+\frac{2m}{\hbar^2}\left[E-v_1\frac{qe^{-2\alpha x}}{p-qe^{-2\alpha x}}+\frac{v_2 pqe^{-2\alpha x}}{(p-qe^{-2\alpha x})^2}\right]\psi_{pq}(x)=0. \tag{4.1}$$

Here, the appropriate transformation is $e^{-2\alpha x} = s$, this converts equation (4.1) to the standard formula (2.1). With the same manner, we can obtain both of the energy eigenvalues and eigenfunctions in the following forms:

$$E_{npq} = -\frac{\hbar^2\alpha^2}{8m}\frac{\left[\sqrt{\frac{2mv_1}{\hbar^2\alpha^2}}-(2n+1)-\sqrt{1+\frac{2mv_2}{\hbar^2\alpha^2}}\right]^2\left[\sqrt{\frac{2mv_1}{\hbar^2\alpha^2}}+(2n+1)+\sqrt{1+\frac{2mv_2}{\hbar^2\alpha^2}}\right]^2}{\left[(2n+1)+\sqrt{1+\frac{2mv_2}{\hbar^2\alpha^2}}\right]^2}, \tag{4.2}$$

$$y_{npq}(s) = B_n s^{-2\sqrt{\varepsilon}}(p-qs)^{-(\mu-1)}\frac{d^n}{ds^n}[s^{n+2\sqrt{\varepsilon}}(p-qs)^{n+(\mu-1)}], \tag{4.3}$$

$$\psi_{npq}(s) = s^{\sqrt{\varepsilon}}(p-qs)^{\frac{\mu}{2}}y_{npq}(s), \tag{4.4}$$

with $\varepsilon = \varepsilon_{npq} = -\dfrac{mE_{npq}}{2\hbar^2\alpha^2}$, $\mu = 1-\sqrt{1+\dfrac{2mv_2}{\hbar^2\alpha^2}}$ and $s = e^{-2\alpha x}$.

Finally, if we consider the potential, then $V_{pq}(x)$ takes the form (1.5). Analogously, we have

$$E_{npq} = \frac{v_1}{2}-\frac{mv_1^2}{2\hbar^2\alpha^2\left[-(2n+1)+\sqrt{1+\frac{2mv_2}{\hbar^2\alpha^2}}\right]^2}-\frac{\hbar^2\alpha^2}{8m}\left[-(2n+1)+\sqrt{1+\frac{2mv_2}{\hbar^2\alpha^2}}\right]^2, \tag{4.5}$$

$$y_{npq}(s) = B_n s^{-2\sqrt{\varepsilon+\frac{mv_1}{2\hbar^2\alpha^2}}}(p-qs)^{-(\mu-1)}\frac{d^n}{ds^n}[s^{n+2\sqrt{\varepsilon+\frac{mv_1}{2\hbar^2\alpha^2}}}(p-qs)^{n+(\mu-1)}], \tag{4.6}$$

$$\psi_{npq}(s) = s^{\sqrt{\varepsilon + \frac{mv_1}{2\hbar^2\alpha^2}}} (p - qs)^{\frac{\mu}{2}} y_{npq}(s), \tag{4.7}$$

with $s = -e^{-2\alpha x}$, we can observe that the previous two cases are correspondence where the deformation parameters p, q are constructive with respect to the wave function. On the other hand, with regard to the energy eigenvalues are independent of these parameters.

5. Summary and Discussion

In conclusion, we have calculated the energy levels and the wave functions of some generalized potentials such as the generalized Rosen-Morse, Pöschl-Teller, generalized modified Rosen-Morse and generalized hyperbolic Kratzer-like potentials by solving the Schrödinger equation. The UN method is used to obtain these quantities. With the purpose of the illustration of the method, four different potentials are introduced for the first time. It is remarkable that the energy eigenvalues for the generalized Rosen-Morse and the generalized Pöschl-Teller potentials depend on the deformation parameters p, q while the generalized hyperbolic Kratzer and modified Rosen-Morse potentials are independent of these parameters. Thus, we can see that the potentials (1.4) and (1.5) are shape invariant potentials, that is to say, the pq-invariant shape of the potential leads to the pq-independent energy eigenvalues.

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