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Research Article

Approximate *l*-States of the Manning-Rosen Potential by Using Nikiforov-Uvarov Method

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The approximately analytical bound state solutions of the l-wave Schrödinger equation for the Manning-Rosen (MR) potential are carried out by a proper approximation to the centrifugal term. The energy spectrum formula and normalized wave functions expressed in terms of the Jacobi polynomials are both obtained for the application of the Nikiforov-Uvarov (NU) method to the Manning-Rosen potential. To show the accuracy of our results, we calculate the eigenvalues numerically for arbitrary principal and orbital quantum numbers n and l with two different values of the potential screening parameter α. It is found that our results are in good agreement with the those obtained by other methods for short potential range, lowest values of orbital quantum number l, and α. Two special cases of much interest are investigated like the s-wave case and Hulthén potential case.

1. Introduction

One of the important tasks of quantum mechanics is to find exact solutions of the wave equations (nonrelativistic and relativistic) for certain type of potentials of physical interest since they contain all the necessary information regarding the quantum system under consideration. For example, the exact solutions of these wave equations are only possible in a few simple cases such as the Coulomb, harmonic oscillator, pseudoharmonic, and Mie-type potentials [1–10]. For an arbitrary l-state, most quantum systems could be only treated by approximation methods. For the rotating Morse potential, some semiclassical and/or numerical solutions have been obtained by using Pekeris approximation [11–15]. In recent years, many authors have studied the nonrelativistic and relativistic wave equations with certain potentials for the s- and l-waves. The exact and approximate solutions of these models have been obtained analytically [12–24].

Many exponential-type potentials have been solved like the Morse potential [14, 18, 21], the Hulthén potential [19, 25–29], the Pöschl-Teller potential [30], the Woods-Saxon potential [31–34], the Kratzer-type potentials [16, 35–44], the Rosen-Morse-type potentials [45, 46], the Manning-Rosen potential [47–52], generalized Morse potential [17, 18], and other multiparameter exponential-type potentials [53, 54]. Various methods are used to obtain the exact solutions of the wave equations for this type of exponential potentials. These methods include the supersymmetric (SUSY) and shape invariant method [28, 29, 55], the variational [56], the path integral approach [49], the standard methods [50–52], the asymptotic iteration method (AIM) [57, 58], the exact quantization rule (EQR) [15, 59–62], the hypervirial perturbation [63], the shifted $1/N$ expansion (SE) [64–75] and the modified shifted $1/N$ expansion (MSE) [76], series method [77], smooth transformation [78], the algebraic approach [79], the perturbative treatment [80–86] and the Nikiforov-Uvarov (NU) method [25–27, 30–43, 87–91], and others. The NU method [91] is based on solving the second-order linear differential equation by reducing to a generalized equation of hypergeometric type. It has been used to solve the Schrödinger [16, 21, 25, 30, 32, 33, 37, 39, 83–85], Dirac [17, 18, 27, 35–38, 45, 87–89], Klein-Gordon [12, 20, 22, 31, 32, 35, 37, 38, 92] wave equations for such kinds of exponential potentials.

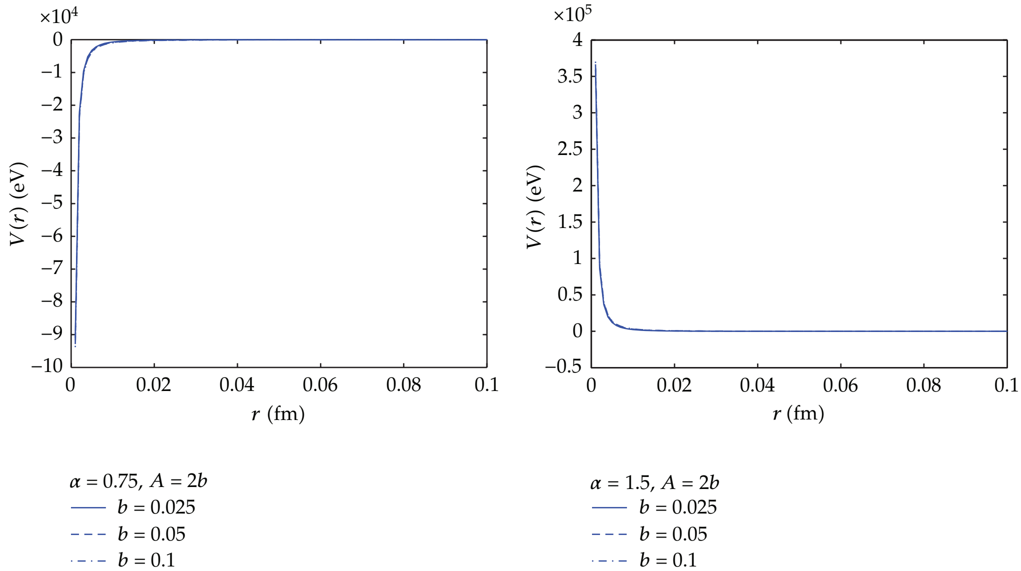
The NU method has shown its power in calculating the exact energy levels of all bound states for some solvable quantum systems. Motivated by the considerable interest in exponential-type potentials [14–19, 24–54], we attempt to study the quantum properties of another exponential-type potential proposed by Manning and Rosen (MR) [46–52]:

$$V(r) = \varepsilon_0\left(\frac{\alpha(\alpha-1)e^{-2r/b}}{\left(1-e^{-r/b}\right)^2} - \frac{Ae^{-r/b}}{1-e^{-r/b}}\right), \quad \varepsilon_0 = \frac{\hbar^2}{2\mu b^2}, \tag{1.1}$$

where A and α are two-dimensionless parameters, but the screening parameter b has dimension of length and corresponds to the potential range [51, 52]. Also, an energy scale ε_0 has been introduced for the potential part. This potential is used as a mathematical model in the description of diatomic molecular vibrations [93, 94], and it constitutes a convenient model for other physical situations. Figure 1 shows the variation of the MR potential (1.1) with r for various screening distances $b = 0.025, 0.050$, and 0.100 considering the cases (a) $\alpha = 0.75$ and (b) $\alpha = 1.50$. It is known that for this potential the Schrödinger equation can be solved exactly for s-wave (i.e., $l = 0$) [50]. Unfortunately, for an arbitrary l-states ($l \neq 0$), the Schrödinger equation does not admit an exact analytic solution. In such a case, the Schrödinger equation is solved numerically [95] or approximately using approximation schemes [19, 23, 88–90, 96–99]. Some authors used the approximation scheme proposed by Greene and Aldrich [19] to study analytically the $l \neq 0$ bound states or scattering states of the Schrödinger or even relativistic wave equations for MR potential [15, 31, 32]. We calculate and find its $l \neq 0$ bound state energy spectrum and normalized wave functions [46–52]. The potential (1.1) may be further put in the following simple form:

$$V(r) = -\frac{Ce^{-r/b} + De^{-2r/b}}{\left(1-e^{-r/b}\right)^2}, \quad C = A, \ D = -A - \alpha(\alpha-1). \tag{1.2}$$

It is also used in several branches of physics for their bound states and scattering properties. Its spectra have already been calculated via Schrö dinger formulation [47, 48]. In our analysis,



(a) (b)

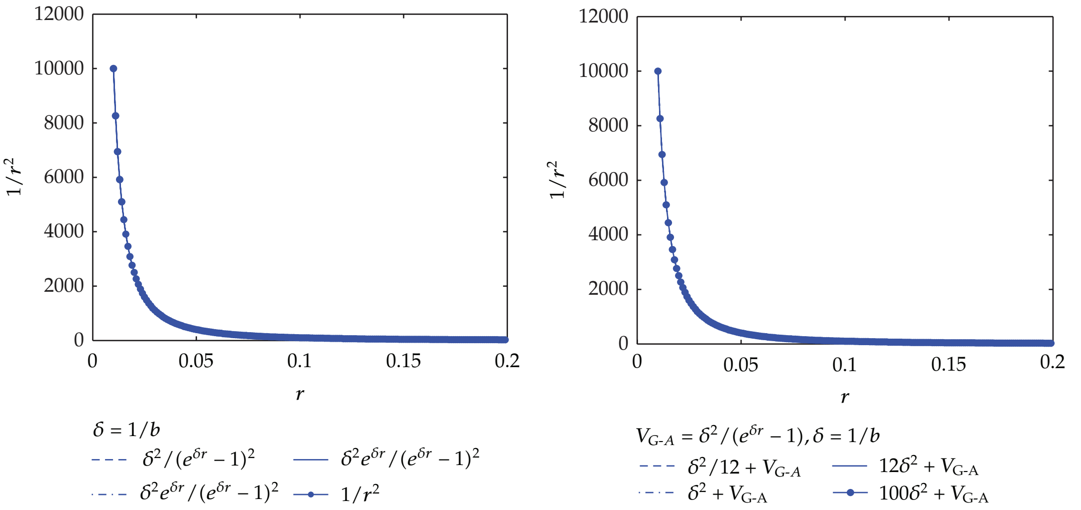
Figure 1: Variation of MR potential as function of separation distance r taking various values for the screening parameter b when (a) $\alpha = 0.75$ and (b) $\alpha = 1.50$.

we find that the potential (1.1) remains invariant by mapping $\alpha \longrightarrow 1 - \alpha$. Further, it has a relative minimum value $V(r_0) = -(A^2/4\kappa b^2\alpha(\alpha - 1))$ at $r_0 = b\ln[1 + (2\alpha(\alpha - 1)/A)]$ for $A/2 + \alpha(\alpha - 1) > 0$ which provides $2\alpha > 1 + \sqrt{1 - 2A}$ as a result of the first derivative $dV/dr|_{r=r_0} = 0$. For the case $\alpha = 0.75$, we have the criteria imposed on the value of A: $A > \alpha/2 = 3/8$. For example, in $\hbar = \mu = 1$, the minimum of the potential is $V(r_0) = -\alpha/16b^2(\alpha - 1)$. The second derivative which determines the force constants at $r = r_0$ is given by

$$\left.\frac{d^2V}{dr^2}\right|_{r=r_0} = \frac{A^2[A + 2\alpha(\alpha - 1)]^2}{8b^4\alpha^3(\alpha - 1)^3}. \tag{1.3}$$

The purpose of this paper is to investigate the l-state solution of the Schrödinger-MR problem within the Nikiforov-Uvarov method to generate accurate energy spectrum. The solution is mainly depending on replacing the orbital centrifugal term of singularity $\sim 1/r^2$ [27] with Greene-Aldrich approximation scheme, consisting of the exponential form [25, 26]. Figure 2 shows the behaviour of the singular term r^{-2} and various approximation schemes recently used in [17–19, 23, 96–98].

sThe paper is organized as follows: in Section 2 we present the shortcuts of the NU method. In Section 3, we derive $l \neq 0$ bound state eigensolutions (energy spectrum and wave functions) of the MR potential by means of the NU method. In Section 4, we give numerical calculations for various diatomic molecules. Section 5 is devoted for discussions. The concluding remarks are given in Section 6.



(a) (b)

Figure 2: A plot of the variation of the singular orbital term $1/r^2$ (dotted-solid line) with the approximations of (a) [17, 18] (dash line), the conventional Greene-Aldrich of [19] (dash-dot line), and improved [23, 96–98] (solid line) replacing the term $1/r^2$ with respect to r, where $\delta = 0.1\,\text{fm}^{-1}$, and (b) the improved approximation [96–98] with various shifting constants.

2. Method

The Nikiforov-Uvarov (NU) method is based on solving the hypergeometric type second order differential equation [91]. Employing an appropriate coordinate transformation $z = z(r)$, we may rewrite the Schrödinger equation in the following form:

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

where $\sigma(z)$ and $\tilde{\sigma}(z)$ are the polynomials with at most of second-degree, and $\tilde{\tau}(s)$ is a first-degree polynomial. Further, using $\psi_n(z) = \phi_n(z)y_n(z)$, (2.1) reduces into an equation of the following hypergeometric type:

$$\sigma(z)y_n''(z) + \tau(z)y_n'(z) + \lambda y_n(z) = 0, \tag{2.2}$$

where $\tau(z) = \tilde{\tau}(z) + 2\pi(z)$ (its derivative must be negative), and λ is a constant given in the form

$$\lambda = \lambda_n = -n\tau'(z) - \frac{n(n-1)}{2}\sigma''(z), \quad n = 0, 1, 2, \ldots. \tag{2.3}$$

It is worthwhile to note that λ or λ_n is obtained from a particular solution of the form $y(z) = y_n(z)$ which is a polynomial of degree n. Further, $y_n(z)$ is the hypergeometric-type function whose polynomial solutions are given by Rodrigues relation:

$$y_n(z) = \frac{B_n}{\rho(z)} \frac{d^n}{dz^n} \left[\sigma^n(z)\rho(z)\right], \tag{2.4}$$

where B_n is the normalization constant, and the weight function $\rho(z)$ must satisfy the condition [91]

$$w'(z) - \left(\frac{\tau(z)}{\sigma(z)}\right) w(z) = 0, \qquad w(z) = \sigma(z)\rho(z). \tag{2.5}$$

In order to determine the weight function given in (2.5), we must obtain the following polynomial:

$$\pi(z) = \frac{\sigma'(z) - \tilde{\tau}(z)}{2} \pm \sqrt{\left(\frac{\sigma'(z) - \tilde{\tau}(z)}{2}\right)^2 - \tilde{\sigma}(z) + k\sigma(z)}. \tag{2.6}$$

In principle, the expression under the square root sign in (2.6) can be arranged as the square of a polynomial. This is possible only if its discriminant is zero. In this case, an equation for k is obtained. After solving this equation, the obtained values of k are included in the NU method and here there is a relationship between λ and k by $k = \lambda - \pi'(z)$. After this point, an appropriate $\phi_n(z)$ can be calculated as the solution of the differential equation:

$$\phi'(z) - \left(\frac{\pi(z)}{\sigma(z)}\right) \phi(z) = 0. \tag{2.7}$$

3. Bound-State Solutions for Arbitrary l-States

To study any quantum physical system characterized by the empirical potential given in (1.1), we solve the original SE which is given in the well-known textbooks [1, 2]

$$\left(\frac{p^2}{2m} + V(r)\right) \psi(\mathbf{r}, \theta, \phi) = E\psi(\mathbf{r}, \theta, \phi), \tag{3.1}$$

where the potential $V(r)$ is taken as the MR form in (1.1). Using the separation method with the wavefunction $\psi(\mathbf{r}, \theta, \phi) = r^{-1}R(r)Y_{lm}(\theta, \phi)$, we obtain the following radial Schrödinger equation:

$$\frac{d^2 R_{nl}(r)}{dr^2} + \left\{\frac{2\mu E_{nl}}{\hbar^2} - \frac{1}{b^2}\left[\frac{\alpha(\alpha - 1)e^{-2r/b}}{\left(1 - e^{-r/b}\right)^2} - \frac{Ae^{-r/b}}{1 - e^{-r/b}}\right] - \frac{l(l+1)}{r^2}\right\} R_{nl}(r) = 0. \tag{3.2}$$

Since the Schrödinger equation with MR effective potential

$$U_{\mathrm{eff}}(x) = \frac{l(l+1)}{x^2} + \left[\frac{\alpha(\alpha-1)e^{-2x}}{(1-e^{-x})^2} - \frac{Ae^{-x}}{1-e^{-x}}\right], \quad x = \frac{r}{b}, \tag{3.3}$$

has no analytical solution for $l \neq 0$ states, an approximation to the centrifugal term has to be made. The good approximation for the too singular kinetic energy term $l(l+1)r^{-2}$ in the centrifugal barrier is taken as [19, 51, 52]

$$\frac{1}{r^2} \approx \frac{1}{b^2}\frac{e^{-r/b}}{\left(1-e^{-r/b}\right)^2}, \tag{3.4}$$

in a short potential range. To solve it by the present method, we need to recast (3.2) with (3.4) into the form of (2.1) by making change of the variables $r \to z$ through the mapping function $r = f(z)$ and energy transformation:

$$z = e^{-r/b}, \qquad \varepsilon = \sqrt{-\frac{2\mu b^2 E_{nl}}{\hbar^2}}, \quad E_{nl} < 0, \tag{3.5}$$

to obtain the following hypergeometric equation:

$$\begin{aligned}\frac{d^2R(z)}{dz^2} &+ \frac{(1-z)}{z(1-z)}\frac{dR(z)}{dz} \\ &+ \frac{1}{[z(1-z)]^2}\left\{-\varepsilon^2 + \left[A + 2\varepsilon^2 - l(l+1)\right]z - \left[A + \varepsilon^2 + \alpha(\alpha-1)\right]z^2\right\}R(z) = 0.\end{aligned} \tag{3.6}$$

It is noted that the bound state (real) solutions of the last equation demand that

$$z = \begin{cases} 0, & \text{when } r \longrightarrow \infty, \\ 1, & \text{when } r \longrightarrow 0, \end{cases} \tag{3.7}$$

and thus provide the finite radial wave functions $R_{nl}(z) \to 0$. To apply the hypergeometric method (NU), it is necessary to compare (3.6) with (2.1). Subsequently, the following value for the parameters in (2.1) is obtained:

$$\tilde{\tau}(z) = 1 - z, \qquad \sigma(z) = z - z^2, \qquad \tilde{\sigma}(z) = -\left[A + \varepsilon^2 + \alpha(\alpha-1)\right]z^2 + \left[A + 2\varepsilon^2 - l(l+1)\right]z - \varepsilon^2. \tag{3.8}$$

If one inserts these values of parameters into (2.6), with $\sigma'(z) = 1 - 2z$, the following linear function is achieved

$$\pi(z) = -\frac{z}{2} \pm \frac{1}{2}\sqrt{a_1 z^2 + a_2 z + a_3}, \tag{3.9}$$

where $a_1 = 1 + 4[A + \varepsilon^2 + \alpha(\alpha - 1) - k]$, $a_2 = 4\{k - [A + 2\varepsilon^2 - l(l + 1)]\}$, and $a_3 = 4\varepsilon^2$. According to this method, the expression in the square root has to be set equal to zero, that is, $\Delta = a_1 z^2 + a_2 z + a_3 = 0$. Thus the constant k can be determined as

$$k = A - l(l+1) \pm a\varepsilon, \qquad a = \sqrt{(1-2\alpha)^2 + 4l(l+1)}. \tag{3.10}$$

In view of that, we can find four possible functions for $\pi(z)$ as

$$\pi(z) = -\frac{z}{2} \pm \begin{cases} \varepsilon - \left(\varepsilon - \dfrac{a}{2}\right)z, & \text{for } k = A - l(l+1) + a\varepsilon, \\ \varepsilon - \left(\varepsilon + \dfrac{a}{2}\right)z, & \text{for } k = A - l(l+1) - a\varepsilon. \end{cases} \tag{3.11}$$

We must select

$$k = A - l(l+1) - a\varepsilon, \qquad \pi(z) = -\frac{z}{2} + \varepsilon - \left(\varepsilon + \frac{a}{2}\right)z, \tag{3.12}$$

in order to obtain the polynomial $\tau(z) = \tilde{\tau}(z) + 2\pi(z)$ having negative derivative as

$$\tau(z) = 1 + 2\varepsilon - (2 + 2\varepsilon + a)z, \qquad \tau'(z) = -(2 + 2\varepsilon + a). \tag{3.13}$$

We can also write the values of $\lambda = k+\pi'(z)$ and $\lambda_n = -n\tau'(z)-(n(n-1)/2)\sigma''(z),\ n = 0,1,2,\ldots$ as

$$\begin{gathered} \lambda = A - l(l+1) - (1+a)\left[\frac{1}{2} + \varepsilon\right], \\ \lambda_n = n(1 + n + a + 2\varepsilon), \quad n = 0,1,2,\ldots, \end{gathered} \tag{3.14}$$

respectively. Letting $\lambda = \lambda_n$ and solving the resulting equation for ε lead to the energy equation

$$\varepsilon = \frac{(n+1)^2 + l(l+1) + (2n+1)\Lambda - A}{2(n+1+\Lambda)}, \quad \Lambda = \frac{-1+a}{2}, \tag{3.15}$$

from which we obtain the discrete energy spectrum formula:

$$E_{nl} = -\frac{\hbar^2}{2\mu b^2}\left[\frac{(n+1)^2 + l(l+1) + (2n+1)\Lambda - A}{2(n+1+\Lambda)}\right]^2, \quad 0 \leq n,\ l < \infty, \tag{3.16}$$

where n denotes the radial quantum number. It is found that Λ remains invariant by mapping $\alpha \to 1 - \alpha$, so do the bound state energies E_{nl}. An important quantity of interest for the MR potential is the critical coupling constant A_c, which is that value of A for which the binding energy of the level in question becomes zero. Furthermore, from (3.16), we have (in atomic units $\hbar = \mu = Z = e = 1$),

$$A_c = (n+1+\Lambda)^2 - \Lambda(\Lambda+1) + l(l+1). \tag{3.17}$$

Next, we turn to the radial wave function calculations. We use $\sigma(z)$ and $\pi(z)$ in (3.8) and (3.12) to obtain

$$\phi(z) = z^{\varepsilon}(1-z)^{\Lambda+1}, \tag{3.18}$$

and weight function

$$\rho(z) = z^{2\varepsilon}(1-z)^{2\Lambda+1}, \tag{3.19}$$

$$y_{nl}(z) = C_n z^{-2\varepsilon}(1-z)^{-(2\Lambda+1)} \frac{d^n}{dz^n}\left[z^{n+2\varepsilon}(1-z)^{n+2\Lambda+1}\right]. \tag{3.20}$$

The functions $y_{nl}(z)$, up to a numerical factor, are in the form of Jacobi polynomials, that is, $y_{nl}(z) \simeq P_n^{(2\varepsilon,2\Lambda+1)}(1-2z)$, and physically hold in the interval $(0 \le r < \infty \to 0 \le z \le 1)$ [100]. Therefore, the radial part of the wave functions can be found by substituting (3.18) and (3.20) into $R_{nl}(z) = \phi(z)y_{nl}(z)$ as

$$R_{nl}(z) = N_{nl} z^{\varepsilon}(1-z)^{1+\Lambda} P_n^{(2\varepsilon,2\Lambda+1)}(1-2z), \tag{3.21}$$

where ε and Λ are given in (3.5) and (3.10) and N_{nl} is a normalization constant. This equation satisfies the requirements; $R_{nl}(z) = 0$ as $z = 0\,(r \to \infty)$ and $R_{nl}(z) = 0$ as $z = 1\,(r = 0)$. Therefore, the wave functions, $R_{nl}(z)$, in (3.21) are valid physically in the closed interval $z \in [0,1]$ or $r \in (0,\infty)$. Further, the wave functions satisfy the normalization condition:

$$\int_0^{\infty} |R_{nl}(r)|^2 dr = 1 = b\int_0^1 z^{-1}|R_{nl}(z)|^2 dz, \tag{3.22}$$

where N_{nl} can be determined via

$$1 = bN_{nl}^2 \int_0^1 z^{2\varepsilon-1}(1-z)^{2\Lambda+2}\left[P_n^{(2\varepsilon,2\Lambda+1)}(1-2z)\right]^2 dz. \tag{3.23}$$

The Jacobi polynomials, $P_n^{(\rho,\nu)}(\xi)$, can be explicitly written in two different ways [101, 102]:

$$\begin{aligned} P_n^{(\rho,\nu)}(\xi) &= 2^{-n}\sum_{p=0}^{n}(-1)^{n-p}\binom{n+\rho}{p}\binom{n+\nu}{n-p}(1-\xi)^{n-p}(1+\xi)^p, \\ P_n^{(\rho,\nu)}(\xi) &= \frac{\Gamma(n+\rho+1)}{n!\Gamma(n+\rho+\nu+1)}\sum_{r=0}^{n}\binom{n}{r}\frac{\Gamma(n+\rho+\nu+r+1)}{\Gamma(r+\rho+1)}\left(\frac{\xi-1}{2}\right)^r, \end{aligned} \tag{3.24}$$

where $\binom{n}{r} = n!/r!(n-r)! = \Gamma(n+1)/\Gamma(r+1)\Gamma(n-r+1)$. After using (3.24), we obtain the explicit expressions for $P_n^{(2\varepsilon,2\Lambda+1)}(1-2z)$:

$$\begin{aligned} P_n^{(2\varepsilon,2\Lambda+1)}(1-2z) &= (-1)^n\Gamma(n+2\varepsilon+1)\Gamma(n+2\Lambda+2) \\ &\quad\times\sum_{p=0}^{n}\frac{(-1)^p}{p!(n-p)!\Gamma(p+2\Lambda+2)\Gamma(n+2\varepsilon-p+1)}z^{n-p}(1-z)^p, \\ P_n^{(2\varepsilon,2\Lambda+1)}(1-2z) &= \frac{\Gamma(n+2\varepsilon+1)}{\Gamma(n+2\varepsilon+2\Lambda+2)}\sum_{r=0}^{n}\frac{(-1)^r\Gamma(n+2\varepsilon+2\Lambda+r+2)}{r!(n-r)!\Gamma(2\varepsilon+r+1)}z^r. \end{aligned} \tag{3.25}$$

Inserting (3.25) into (3.23), one obtains

$$\begin{aligned} 1 &= bN_{nl}^2(-1)^n\frac{\Gamma(n+2\Lambda+2)\Gamma(n+2\varepsilon+1)^2}{\Gamma(n+2\varepsilon+2\Lambda+2)} \\ &\quad\times\sum_{p,r=0}^{n}\frac{(-1)^{p+r}\Gamma(n+2\varepsilon+2\Lambda+r+2)}{p!r!(n-p)!(n-r)!\Gamma(p+2\Lambda+2)\Gamma(n+2\varepsilon-p+1)\Gamma(2\varepsilon+r+1)}I_{nl}(p,r), \end{aligned} \tag{3.26}$$

where

$$I_{nl}(p,r) = \int_0^1 z^{n+2\varepsilon+r-p-1}(1-z)^{p+2\Lambda+2}dz. \tag{3.27}$$

The following integral representation of the hypergeometric function [101, 102]

$${}_2F_1(\alpha_0,\beta_0:\gamma_0;1)\frac{\Gamma(\alpha_0)\Gamma(\gamma_0-\alpha_0)}{\Gamma(\gamma_0)} = \int_0^1 z^{\alpha_0-1}(1-z)^{\gamma_0-\alpha_0-1}(1-z)^{-\beta_0}dz, \qquad \gamma_0>\alpha_0>0, \tag{3.28}$$

gives

$$\frac{{}_2F_1(\alpha_0,\beta_0:\alpha_0+1;1)}{\alpha_0} = \int_0^1 z^{\alpha_0-1}(1-z)^{-\beta_0}dz, \tag{3.29}$$

where

$${}_2F_1(\alpha_0,\beta_0:\gamma_0;1) = \frac{\Gamma(\gamma_0)\Gamma(\gamma_0-\alpha_0-\beta_0)}{\Gamma(\gamma_0-\alpha_0)\Gamma(\gamma_0-\beta_0)}, \quad \gamma_0-\alpha_0-\beta_0>0,\ \gamma_0>\beta_0>0. \tag{3.30}$$

For the present case, with the aid of (3.28), when $\alpha_0 = n+2\varepsilon+r-p$, $\beta_0 = -p-2\Lambda-2$, and $\gamma_0 = \alpha_0+1$ are substituted into (3.29), we obtain

$$I_{nl}(p,r) = \frac{{}_2F_1(\alpha_0,\beta_0:\gamma_0;1)}{\alpha_0} = \frac{\Gamma(n+2\varepsilon+r-p+1)\Gamma(p+2\Lambda+3)}{(n+2\varepsilon+r-p)\Gamma(n+2\varepsilon+r+2\Lambda+3)}. \tag{3.31}$$

Finally, we obtain

$$\begin{aligned}1 = bN_{nl}^2(-1)^n\frac{\Gamma(n+2\Lambda+2)\Gamma(n+2\varepsilon+1)^2}{\Gamma(n+2\varepsilon+2\Lambda+2)}\\ \times\sum_{p,r=0}^{n}\frac{(-1)^{p+r}\Gamma\left(n+2\varepsilon+r-p+1\right)\left(p+2\Lambda+2\right)}{p!r!(n-p)!(n-r)!\Gamma\left(n+2\varepsilon-p+1\right)\Gamma(2\varepsilon+r+1)(n+2\varepsilon+r+2\Lambda+2)},\end{aligned} \tag{3.32}$$

which gives

$$N_{nl} = \frac{1}{\sqrt{s(n)}}, \tag{3.33}$$

where

$$\begin{aligned}s(n) = b(-1)^n\frac{\Gamma(n+2\Lambda+2)\Gamma(n+2\varepsilon+1)^2}{\Gamma(n+2\varepsilon+2\Lambda+2)}\\ \times\sum_{p,r=0}^{n}\frac{(-1)^{p+r}\Gamma\left(n+2\varepsilon+r-p+1\right)\left(p+2\Lambda+2\right)}{p!r!(n-p)!(n-r)!\Gamma\left(n+2\varepsilon-p+1\right)\Gamma(2\varepsilon+r+1)(n+2\varepsilon+r+2\Lambda+2)}.\end{aligned} \tag{3.34}$$

4. Numerical Results

To show the accuracy of our results, we calculate the energy eigenvalues for various n and l quantum numbers with two different values of the parameters α. It is shown in Table 1 that the present approximately numerical results are not in a good agreement for the long potential range (high screening regime). The energy eigenvalues for short potential range (large values of parameter b) are in agreement with the other authors. The energy spectra for various diatomic molecules like HCl, CH, LiH, and CO are presented in Tables 2 and 3. These results are relevant to atomic physics [103–108], molecular physics [109, 110], and chemical physics [111, 112], and so forth.

5. Discussions

In this work, we have utilized the hypergeometric method and solved the radial SE for the MR model potential with the angular momentum $l \neq 0$ states. We have derived the binding energy spectra in (3.16) and their corresponding wave functions in (3.21).

Let us study special cases. We have shown that inserting $\alpha = 0$ in (1.1), the present solution reduces to the one of the Hulthén potential [25, 26, 28, 29, 99]:

$$V^{(H)}(r) = -V_0\frac{e^{-\delta r}}{1-e^{-\delta r}}, \quad V_0 = Ze^2\delta,\ \delta = b^{-1}, \tag{5.1}$$

where Ze^2 is the potential strength parameter and δ is the screening parameter and b is the range of potential. We note also that it is possible to recover the Yukawa potential by letting

Table 1: Energies (in atomic units) of different n and l states and for $\alpha = 0.75$ and $\alpha = 1.5$, $A = 2b$.

			$\alpha = 0.75$			$\alpha = 1.5$	
States	$1/b$	Present	QD [51, 52]	LS [95]	Present	QD [51, 52]	LS [95]
$2p$	0.025	−0.1205793	−0.1205793	−0.1205271	−0.0900228	−0.0900229	−0.0899708
	0.050	−0.1084228	−0.1084228	−0.1082151	−0.0802472	−0.0802472	−0.0800400
	0.075	−0.0969120	−0.0969120	−0.0964469	−0.0710332	−0.0710332	−0.0705701
	0.100	−0.0860740			−0.0577157		
$3p$	0.025	−0.0459296	−0.0459297	−0.0458779	−0.0369650	−0.0369651	−0.0369134
	0.050	−0.0352672	−0.0352672	−0.0350633	−0.0274719	−0.0274719	−0.0272696
	0.075	−0.0260109	−0.0260110	−0.0255654	−0.0193850	−0.0193850	−0.0189474
	0.100	−0.0181609			−0.0127043		
$3d$	0.025	−0.0449299	−0.0449299	−0.0447743	−0.0396344	−0.0396345	−0.0394789
	0.050	−0.0343082	−0.0343082	−0.0336930	−0.0300629	−0.0300629	−0.0294496
	0.075	−0.0251168	−0.0251168	−0.0237621	−0.0218120	−0.0218121	−0.0204663
$4p$	0.025	−0.0208608	−0.0208608	−0.0208097	−0.0172249	−0.0172249	−0.0171740
	0.050	−0.0119291	−0.0119292	−0.0117365	−0.0091019	−0.0091019	−0.0089134
	0.075	−0.0054773	−0.0054773	−0.0050945	−0.0035478	−0.0035478	−0.0031884
$4d$	0.025	−0.0204555	−0.0204555	−0.0203017	−0.0183649	−0.0183649	−0.0182115
	0.050	−0.0115741	−0.0115742	−0.0109904	−0.0100947	−0.0100947	−0.0095167
	0.075	−0.0052047	−0.0052047	−0.0040331	−0.0042808	−0.0042808	−0.0031399
$4f$	0.025	−0.0202886	−0.0202887	−0.0199797	−0.0189222	−0.0189223	−0.0186137
	0.050	−0.0114283	−0.0114284	−0.0102393	−0.0105852	−0.0105852	−0.0094015
	0.075	−0.0050935	−0.0050935	−0.0026443	−0.0046527	−0.0046527	−0.0022307
$5p$	0.025	−0.0098576	−0.0098576	−0.0098079	−0.0081308	−0.0081308	−0.0080816
$5d$	0.025	−0.0096637	−0.0096637	−0.0095141	−0.0086902	−0.0086902	−0.0085415
$5f$	0.025	−0.0095837	−0.0095837	−0.0092825	−0.0089622	−0.0089622	−0.0086619
$5g$	0.025	−0.0095398	−0.0095398	−0.0090330	−0.0091210	−0.0091210	−0.0086150
$6p$	0.025	−0.0044051	−0.0044051	−0.0043583	−0.0035334	−0.0035334	−0.0034876
$6d$	0.025	−0.0043061	−0.0043061	−0.0041650	−0.0038209	−0.0038209	−0.0036813
$6f$	0.025	−0.0042652	−0.0042652	−0.0039803	−0.0039606	−0.0039606	−0.0036774
$6g$	0.025	−0.0042428	−0.0042428	−0.0037611	−0.0040422	−0.0040422	−0.0035623

$b \to \infty$ and $V_0 = Ze^2/b$. If the potential is used for atoms, the Z is identified with the atomic number. This can be achieved by setting $\Lambda = l$, hence, the energy for $l \neq 0$ states

$$E_{nl} = -\frac{\left[A - (n+l+1)^2\right]^2 \hbar^2}{8\mu b^2 (n+l+1)^2}, \quad 0 \leq n,\ l < \infty, \tag{5.2}$$

and for s-wave ($l = 0$) states

$$E_n = -\frac{\left[A - (n+1)^2\right]^2 \hbar^2}{8\mu b^2 (n+1)^2}, \quad 0 \leq n < \infty. \tag{5.3}$$

Table 2: Energy spectrum of HCl and CH (in eV) for different states where $\hbar c = 1973.29\,\text{eV Å}$, $\mu_{\text{HCl}} = 0.9801045\,\text{amu}$, $\mu_{\text{CH}} = 0.929931\,\text{amu}$, and $A = 2b$.

States	$1/b$[a]	HCl/$\alpha = 0, 1$	$\alpha = 0.75$	$\alpha = 1.5$	CH/$\alpha = 0, 1$	$\alpha = 0.75$	$\alpha = 1.5$
$2p$	0.025	−4.81152646	−5.14278553	−3.83953094	−5.07112758	−5.42025940	−4.04668901
	0.050	−4.31837832	−4.62430290	−3.42259525	−4.55137212	−4.87380256	−3.60725796
	0.075	−3.85188684	−4.13335980	−3.02961216	−4.05971155	−4.35637111	−3.19307186
	0.100	−3.41205201	−3.66996049	−2.46161213	−3.59614587	−3.86796955	−2.59442595
$3p$	0.025	−1.86633700	−1.95892730	−1.57658128	−1.96703335	−2.06461927	−1.66164415
	0.050	−1.42316902	−1.50416901	−1.17169439	−1.49995469	−1.58532495	−1.23491200
	0.075	−1.03998066	−1.10938179	−0.82678285	−1.09609178	−1.16923738	−0.87139110
	0.100	−0.71676763	−0.77457419	−0.54184665	−0.75544012	−0.81636557	−0.57108145
$3d$	0.025	−1.86633700	−1.91628944	−1.69043293	−1.96703335	−2.01968093	−1.78163855
	0.050	−1.42316902	−1.46326703	−1.28220223	−1.49995469	−1.54221615	−1.35138217
	0.075	−1.03998066	−1.07124785	−0.93029598	−1.09609178	−1.12904596	−0.98048917
	0.100	−0.71676763	−0.74022762	−0.63472271	−0.75544012	−0.78016587	−0.66896854
$4p$	0.025	−0.85301300	−0.88972668	−0.73465318	−0.89903647	−0.93773100	−0.77429066
	0.050	−0.47981981	−0.50878387	−0.38820195	−0.50570801	−0.53623480	−0.40914700
	0.075	−0.21325325	−0.23361041	−0.15131598	−0.22475912	−0.24621462	−0.15948008
$4d$	0.025	−0.85301300	−0.87244037	−0.78327492	−0.89903647	−0.91951202	−0.82553574
	0.050	−0.47981981	−0.49364289	−0.43054552	−0.50570801	−0.52027690	−0.45377517
	0.075	−0.21325325	−0.22198384	−0.18257890	−0.22475912	−0.23396076	−0.19242977
$4f$	0.025	−0.85301300	−0.86532198	−0.80704413	−0.89903647	−0.91200956	−0.85058739
	0.050	−0.47981981	−0.48742442	−0.45146566	−0.50570801	−0.51372292	−0.47582404
	0.075	−0.21325325	−0.21724109	−0.19844068	−0.22475912	−0.22896211	−0.20914735
$5p$	0.025	−0.40318193	−0.42043305	−0.34678391	−0.42493521	−0.44311709	−0.36549429
$5d$	0.025	−0.40318193	−0.41216309	−0.37064268	−0.42493521	−0.43440094	−0.39064034
$5f$	0.025	−0.40318193	−0.40875104	−0.38224366	−0.42493521	−0.43080479	−0.40286723
$5g$	0.025	−0.40318193	−0.40687867	−0.38901658	−0.42493521	−0.42883140	−0.41000558
$6p$	0.025	−0.17919244	−0.18788038	−0.15070181	−0.18886059	−0.19801728	−0.15883277
$6d$	0.025	−0.17919244	−0.18365796	−0.16296387	−0.18886059	−0.19356705	−0.17175642
$6f$	0.025	−0.17919244	−0.18191355	−0.16892216	−0.18886059	−0.19172852	−0.17803620
$6g$	0.025	−0.17919244	−0.18095818	−0.17240246	−0.18886059	−0.19072160	−0.18170426

[a] b is in pm.

Essentially, these results coincide with those obtained by the Feynman integral method [23, 49] and the standard way [50–52], respectively. Furthermore, if taking $b = 1/\delta$ and identifying $A\hbar^2/2\mu b^2$ as $Ze^2\delta$, we are able to obtain

$$E_{nl} = -\frac{\mu\left(Ze^2\right)^2}{2\hbar^2}\left[\frac{1}{n+l+1} - \frac{\hbar^2\delta}{2Ze^2\mu}(n+l+1)\right]^2, \tag{5.4}$$

which coincides with those of [25, 26, 28, 29]. Further, we have (in atomic units $\hbar = \mu = Z = e = 1$)

$$E_{nl} = -\frac{1}{2}\left[\frac{1}{n+l+1} - \frac{(n+l+1)}{2}\delta\right]^2, \tag{5.5}$$

which coincides with [25, 26, 51, 52].

Table 3: Energy spectrum of LiH and CO (in eV) for different states where $\hbar c = 1973.29\,\text{eV Å}$, $\mu_{\text{LiH}} = 0.8801221\,\text{amu}$, $\mu_{\text{CO}} = 6.8606719\,\text{amu}$, and $A = 2b$.

States	$1/b$[a]	LiH/$\alpha = 0, 1$	$\alpha = 0.75$	$\alpha = 1.5$	CO/$\alpha = 0, 1$	$\alpha = 0.75$	$\alpha = 1.5$
$2p$	0.025	−5.35811876	−5.72700906	−4.27570397	−1.374733789	−0.734690030	−0.548509185
	0.050	−4.80894870	−5.14962650	−3.81140413	−1.233833096	−0.660620439	−0.488946426
	0.075	−4.28946350	−4.60291196	−3.37377792	−1.100548657	−0.590485101	−0.432805497
	0.100	−3.79966317	−4.08687021	−2.74125274	−0.974880471	−0.524284624	−0.351661930
$3p$	0.025	−2.07835401	−2.18146262	−1.75568186	−0.533243776	−0.279849188	−0.225227854
	0.050	−1.58484188	−1.67504351	−1.30479958	−0.406623254	−0.214883153	−0.167386368
	0.075	−1.15812308	−1.23540823	−0.92070588	−0.297139912	−0.158484490	−0.118112862
	0.100	−0.79819287	−0.86256629	−0.60340076	−0.204792531	−0.110654417	−0.077407337
$3d$	0.025	−2.07835401	−2.13398108	−1.88246712	−0.533243776	−0.273758013	−0.241492516
	0.050	−1.58484188	−1.62949505	−1.42786117	−0.406623254	−0.209039964	−0.183173338
	0.075	−1.15812308	−1.19294225	−1.03597816	−0.299139912	−0.153036736	−0.132900580
	0.100	−0.79819287	−0.82431793	−0.70682759	−0.204792531	−0.105747722	−0.090675460
$4p$	0.025	−0.94991579	−0.99080017	−0.81811023	−0.243720118	−0.127104916	−0.104951366
	0.050	−0.53432763	−0.56658202	−0.43230193	−0.137092566	−0.072684041	−0.055457903
	0.075	−0.23747895	−0.26014869	−0.16850556	−0.060930029	−0.033373205	−0.021616756
$4d$	0.025	−0.94991579	−0.97155012	−0.87225543	−0.243720118	−0.124635422	−0.111897390
	0.050	−0.53432763	−0.54972102	−0.47945575	−0.137092566	−0.070521025	−0.061507037
	0.075	−0.23747895	−0.24720134	−0.20331998	−0.060930029	−0.031712252	−0.026082927
$4f$	0.025	−0.94991579	−0.96362308	−0.89872483	−0.243720118	−0.123618500	−0.115293020
	0.050	−0.53432763	−0.54279613	−0.50275243	−0.137092566	−0.069632666	−0.064495655
	0.075	−0.23747895	−0.24191980	−0.22098366	−0.060930029	−0.031034710	−0.028348915
$5p$	0.025	−0.44898364	−0.46819450	−0.38617877	−0.115195837	−0.060062386	−0.049540988
$5d$	0.025	−0.44898364	−0.45898506	−0.41274791	−0.115195837	−0.058880953	−0.052949414
$5f$	0.025	−0.44898364	−0.45518540	−0.42566677	−0.115195837	−0.058393512	−0.054606711
$5g$	0.025	−0.44898364	−0.45310033	−0.43320910	−0.115195837	−0.058126029	−0.055574280
$6p$	0.025	−0.19954881	−0.20922370	−0.16782162	−0.051198285	−0.026840287	−0.021529017
$6d$	0.025	−0.19954881	−0.20452162	−0.18147666	−0.051198285	−0.026237080	−0.023280755
$6f$	0.025	−0.19954881	−0.20257904	−0.18811182	−0.051198285	−0.025987876	−0.024131947
$6g$	0.025	−0.19954881	−0.20151514	−0.19198748	−0.051198285	−0.025851393	−0.024629136

[a] b is in pm.

The corresponding radial wave functions are expressed as

$$R_{nl}(r) = N_{nl} e^{-\delta \varepsilon r} \left(1 - e^{-\delta r}\right)^{l+1} P_n^{(2\varepsilon, 2l+1)} \left(1 - 2e^{-\delta r}\right), \tag{5.6}$$

where

$$\varepsilon = \frac{\mu Z e^2}{\hbar^2 \delta} \left[\frac{1}{n + l + 1} - \frac{\hbar^2 \delta}{2 Z e^2 \mu} (n + l + 1) \right], \quad 0 \leq n,\ l < \infty, \tag{5.7}$$

which coincides for the ground state with that given in (2.3) by Greene and Aldrich [19]. In addition, for $\delta r \ll 1$ (i.e., $r/b \ll 1$), the Hulthén potential turns to become a Coulomb potential: $V(r) = -Ze^2/r$ with energy levels and wave functions:

$$\begin{gathered} E_{nl} = -\frac{\varepsilon_0}{(n+l+1)^2}, \quad n = 0, 1, 2, \ldots \\ \varepsilon_0 = \frac{Z^2\hbar^2}{2\mu a_0^2}, \qquad a_0 = \frac{\hbar^2}{\mu e^2}, \end{gathered} \tag{5.8}$$

where $\varepsilon_0 = 13.6\,\text{eV}$ and a_0 is Bohr radius for the Hydrogen atom. The wave functions are

$$R_{nl} = N_{nl} \exp\left[-\frac{\mu Z e^2}{\hbar^2}\frac{r}{(n+l+1)}\right] r^{l+1} P_n^{(2\mu Z e^2/\hbar^2\delta(n+l+1),2l+1)}(1+2\delta r) \tag{5.9}$$

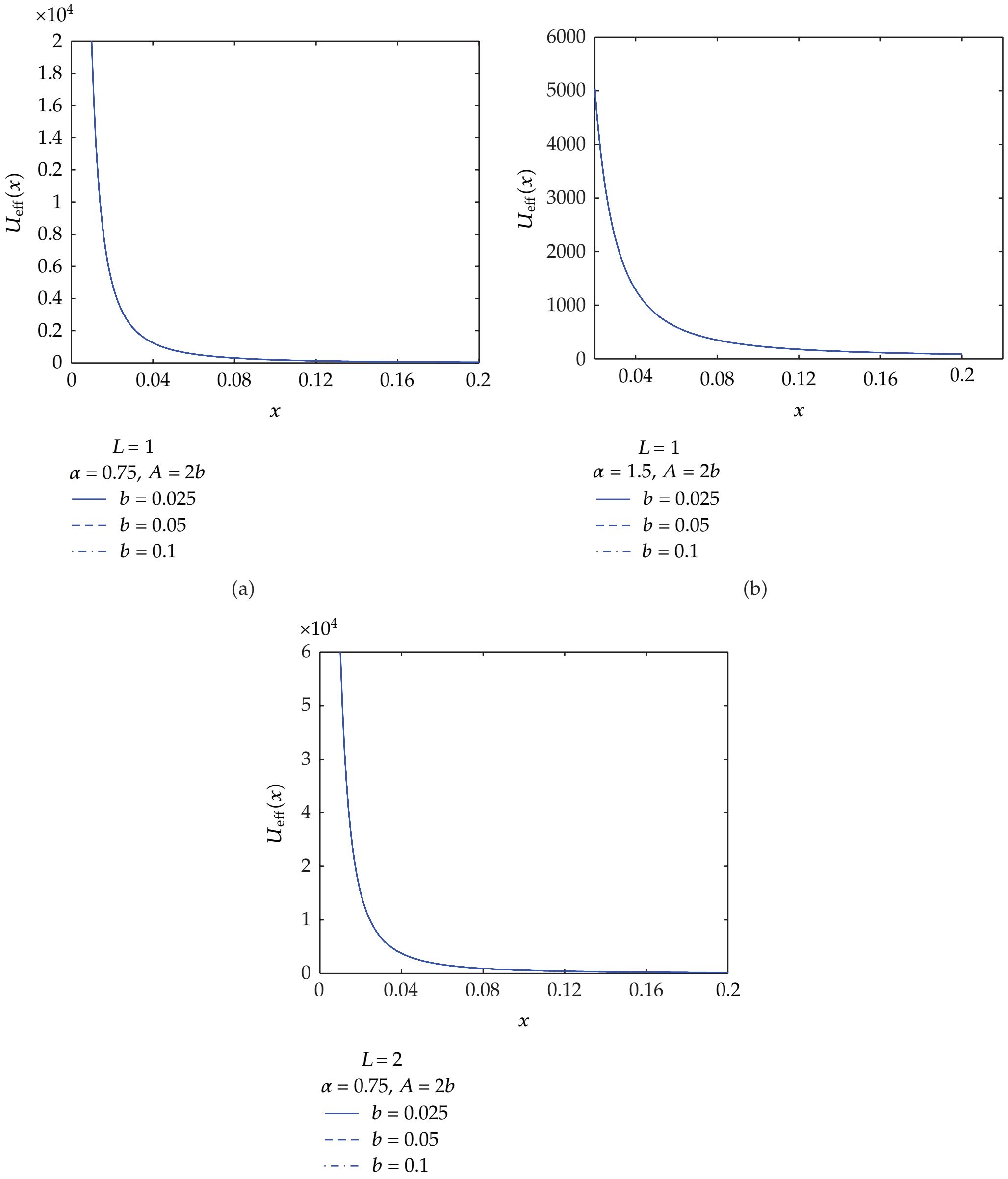
which coincide with [3, 25, 26, 33].

6. Concluding Remarks

In this work, approximate analytical bound states for the l-wave Schrödinger equation with the MR potential have been presented by making a proper approximation to the too singular orbital centrifugal term $\sim r^{-2}$. The normalized radial wave functions of l-wave bound states associated with the MR potential are obtained. The approach enables one to find the l-dependent solutions and the corresponding energy eigenvalues for different screening parameters of the MR potential.

We have shown that for $\alpha = 0, 1$, the present solution reduces to the one of the Hulthén potential. We note that it is possible to recover the Yukawa potential by letting $b \to \infty$ and $V_0 = Ze^2/b$. The Hulthén potential behaves like the Coulomb potential near the origin (i.e., $r \to 0$) $V_C(r) = -Ze^2/r$ but decreases exponentially in the asymptotic region when $r \gg 0$, so its capacity for bound states is smaller than the Coulomb potential [25, 26]. Obviously, the results are in good agreement with those obtained by other methods for short potential range, low values of α, and l. We have also studied two special cases for $l = 0$, $l \neq 0$ and Hulthén potential. The results we have ended up show that the NU method constitutes a reliable alternative way in solving the exponential potentials. We have also found that the criteria for the choice of parameter A require that A satisfies the inequality $\sqrt{1-2A} < 2\alpha - 1$. This means that for real bound state solutions A should be chosen properly in our numerical calculations.

A slight difference in the approximations of the numerical energy spectrum of Schrödinger-MR problem is found in [23, 96–98] and present work since the approximation schemes are different by a small shift $\delta^2/12$. In Figure 2, we plot the variation of the singular orbital term $1/r^2$ (dotted-solid line) with the approximations of (a) [17, 18] (dash line), the conventional Greene-Aldrich of [19] (dash-dot line) and improved [23, 96–98] (solid line) replacing the term $1/r^2$ with respect to r, where $\delta = 0.1\,\text{fm}^{-1}$, and (b) the improved approximation [96–98] with various shifting constants. Figure 2 demonstrates the slight difference between various approximation schemes and the centrifugal term r^{-2}. Further, Figure 3 plots the variations of the effective MR potential as function of separation distance



(a)

(b)

(c)

Figure 3: Variations of the effective MR potential as function of separation distance x taking various values for the screening parameter b when (a) $\alpha = 0.75$, $l = 1$; (b) $\alpha = 1.50$, $l = 1$; (c) $\alpha = 0.75$, $l = 2$; and (d) $\alpha = 1.50$, $l = 2$.

x taking various values for the screening parameter b when (a) $\alpha = 0.75$, $l = 1$; (b) $\alpha = 1.50$, $l = 1$; (c) $\alpha = 0.75$, $l = 2$; and (d) $\alpha = 1.50$, $l = 2$.

In our recent work [27], we have found that the physical quantities like the energy spectrum are critically dependent on the behavior of the system near the singularity ($r = 0$).

That is why, for example, the energy spectrum depends strongly on the angular momentum l, which results from the r^{-2} singularity of the orbital term, even for high excited states. It is found that the r^{-2} orbital term has strong singularity near $r = 0$, then the validity of all such approximations is limited only to very few of the lowest energy states. In this case, to extend accuracy to higher energy states one may attempt to utilize the full advantage of the unique features of Schrödinger equation. Therefore, it is more fruitful to perform the analytic approximation of the less singularity r^{-1} rather than the too singular term r^{-2} which makes it possible to extend the validity of the results to higher excitation levels giving better analytic approximation for a wider energy spectrum [113].

In the meantime after submitting the present work, a recent paper has been published [114] discussing the status of art and the quality of our approximation scheme which has been proposed in [99] and applied recently to MR potential in [115] to calculate the energy spectrum. Stanek [114] used a new improved approximation scheme of the centrifugal term $l(l+1)r^{-2}$ which was proposed by Badawi et al. [116]. This based on the use of the centrifugal term in the form formally homogenous to the original potential to keep the factorizability of the corresponding Schrödinger equation.

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