Approximate $l$-state solutions of the Manning-Rosen potential by the Nikiforov-Uvarov method

Sameer M. Ikhdair* and Ramazan Sever†

*Department of Physics, Near East University, Nicosia, Cyprus, Mersin 10, Turkey.
†Department of Physics, Middle East Technical University, 06531 Ankara, Turkey.

(February 3, 2008)

Abstract

The Schrödinger equation for the Manning-Rosen potential with the centrifugal term is solved approximately to obtain bound states energies. Additionally, the corresponding wave functions are expressed by the Jacobi polynomials. The Nikiforov-Uvarov (NU) method is used in the calculations. To show the accuracy of our results, we calculate the eigenvalues numerically for arbitrary quantum numbers $n$ and $l$ with two different values of the potential parameter $\alpha$. It is shown that the results are in good agreement with the those obtained by other methods for short potential range, small $l$ and $\alpha$. This solution reduces to two cases $l = 0$ and Hulthén potential case.

Keywords: Bound states; Manning-Rosen potential; Nikiforov-Uvarov method.

PACS NUMBER(S): 03.65.-w; 02.30.Gp; 03.65.Ge; 34.20.Cf

*sameer@neu.edu.tr
†sever@metu.edu.tr
I. INTRODUCTION

One of the important tasks of quantum mechanics is to find exact solutions of the wave equations (nonrelativistic and relativistic) for certain potentials of physical interest since they contain all the necessary information regarding the quantum system under consideration. It is well known that the exact solutions of these wave equations are only possible in a few simple cases such as the Coulomb, the harmonic oscillator, pseudoharmonic and Mie-type potentials [1-8]. 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 [9-13]. In recent years, many authors have studied the nonrelativistic and relativistic wave equations for certain potentials for the \( s \)- and \( l \)-cases. The exact and approximate solutions of these models have been obtained analytically [10-14].

Many exponential-type potentials have been solved like the Morse potential [12,13,15], the Hulthén potential [16-19], the Pöschl-Teller [20], the Woods-Saxon potential [21-23], the Kratzer-type potentials [12,14,24-27], the Rosen-Morse-type potentials [28,29], the Manning-Rosen potential [29-33] and other multiparameter exponential-type potentials [34,35]. 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 [19,36], the variational [37], the path integral approach [31], the standard methods [32,33], the asymptotic iteration method (AIM) [38], the exact quantization rule (EQR) [13,39,40], the hypervirial perturbation [41], the shifted \( 1/N \) expansion (SE) [42] and the modified shifted \( 1/N \) expansion (MSE) [43], series method [44], smooth transformation [45], the algebraic approach [46], the perturbative treatment [47,48] and the Nikiforov and Uvarov (NU) method [16,17,20–26,49-51] and others. The NU method [51] 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 [14,16,20,22,49], Dirac [50], Klein-Gordon [17,21,24,25] wave equations for such kinds of exponential potentials.
Recently, the NU method has shown its power in calculating the exact energy levels of all bound states for some solvable quantum systems. In this work, we attempt to apply this method to study another exponential-type potential proposed by Manning and Rosen [29-33]. With an approximation to centrifugal term, we solve the Schrödinger equation to its bound states energies and wavefunctions. This potential is defined as [29-33]

\[
V(r) = -V_0 \frac{e^{-r/b}}{1 - e^{-r/b}} + V_1 \left( \frac{e^{-r/b}}{1 - e^{-r/b}} \right)^2, \quad V_0 = \frac{A}{\kappa b^2}, \quad V_1 = \frac{\alpha (\alpha - 1)}{\kappa b^2}, \quad \kappa = 2\mu/\hbar^2, \tag{1}
\]

where \(A\) and \(\alpha\) are two-dimensionless parameters [27,28] but the screening parameter \(b\) has dimension of length which has a potential range \(1/b\). The potential (1) may be further put in the following simple form

\[
V(r) = -Ce^{-r/b} + De^{-2r/b} \frac{1 - e^{-r/b}}{(1 - e^{-r/b})^2}, \quad C = A, \quad D = -A - \alpha (\alpha - 1), \tag{2}
\]

which is usually used for the description of diatomic molecular vibrations [52,53]. It is also used in several branches of physics for their bound states and scattering properties. The potential in (1) remains invariant by mapping \(\alpha \to 1 - \alpha\) and has a relative minimum value \(V(r_0) = -\frac{A^2}{4kB^2[\alpha (\alpha - 1)]}\) at \(r_0 = b\ln \left[ 1 + \frac{2\alpha (\alpha - 1)}{A} \right]\) for \(\alpha > 0\) to be obtained from the first derivative \(\left. \frac{dV}{dr} \right|_{r=r_0} = 0\). The second derivative which determines the force constants at \(r = r_0\) is given by

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

The contents of this paper are as follows: In Section II we briefly present the Nikiforov-Uvarov (NU) method. In Section III, we derive \(l \neq 0\) bound state eigensolutions (eigenvalues and eigenfunctions) of the Manning-Rosen potential by this method. In Section IV, we present our numerical calculations for various diatomic molecules. Section V, is devoted to for two special cases, namely, \(l = 0\) and the Hulthén potential. The concluding remarks are given in Section VI.
II. THE NIKIFOROV-UVAROV METHOD

The NU method is based on solving the second-order linear differential equation by reducing it to a generalized equation of hypergeometric type [51]. In this method after employing an appropriate coordinate transformation \( z = z(r) \), the Schrödinger equation can be written in the following form:

\[
\psi''_n(z) + \frac{\tilde{\tau}(z)}{\sigma(z)} \psi'_n(z) + \frac{\tilde{\sigma}(z)}{\sigma^2(z)} \psi_n(z) = 0,
\]

(4)

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. The special orthogonal polynomials [51] reduce Eq. (4) to a simple form by employing \( \psi_n(z) = \phi_n(z)y_n(z) \), and choosing an appropriate function \( \phi_n(z) \). Consequently, Eq. (4) can be reduced into an equation of the following hypergeometric type:

\[
\sigma(z)y''_n(z) + \tau(z)y'_n(z) + \lambda y_n(z) = 0,
\]

(5)

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

\[
\lambda = \lambda_n = -n\tau'(z) - \frac{n(n - 1)}{2} \sigma''(z), \quad n = 0, 1, 2, ...
\]

(6)

It is worthwhile to note that \( \lambda \) or \( \lambda_n \) are 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

\[
y_n(z) = \frac{B_n}{\rho(z)} \frac{d^n}{dz^n} [\sigma^n(z)\rho(z)],
\]

(7)

where \( B_n \) is the normalization constant and the weight function \( \rho(z) \) must satisfy the condition [51]

\[
\frac{d}{dz} w(z) = \frac{\tau(z)}{\sigma(z)} w(z), \quad w(z) = \sigma(z)\rho(z).
\]

(8)

In order to determine the weight function given in Eq. (8), we must obtain the following polynomial:
\[
\pi(z) = \frac{\sigma'(z) - \tilde{\tau}(z)}{2} \pm \sqrt{\left(\frac{\sigma'(z) - \tilde{\tau}(z)}{2}\right)^2 - \tilde{\sigma}(z) + k\sigma(z)}.
\] (9)

In principle, the expression under the square root sign in Eq. (9) 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 \(\lambda\) and \(k\) by \(k = \lambda - \pi'(z)\). After this point an appropriate \(\phi_n(z)\) can be extracted from the condition

\[
\frac{\phi'(z)}{\phi(z)} = \frac{\pi(z)}{\sigma(z)}.
\] (10)

### III. BOUND-STATE SOLUTIONS FOR ARBITRARY \(L\)-STATE

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

\[
\left(\frac{p^2}{2m} + V(r)\right) \psi(r,\theta,\phi) = E\psi(r,\theta,\phi),
\] (11)

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

\[
\frac{d^2 R_{nl}(r)}{dr^2} + \left[\frac{2\mu E_{nl}}{\hbar^2} - V_{eff}(r)\right] R_{nl}(r) = 0,
\]

\[
V_{eff}(r) = \frac{1}{b^2} \left[ \frac{\alpha(\alpha-1)e^{-2r/b}}{(1-e^{-r/b})^2} - \frac{Ae^{-r/b}}{1-e^{-r/b}} \right] + \frac{l(l+1)}{r^2}.
\] (12)

Since the Schrödinger equation with above Manning-Rosen effective potential has no analytical solution for \(l \neq 0\) states, an approximation to the centrifugal term has to be made. The good approximation for \(1/r^2\) in the centrifugal barrier is taken as [18,33]

\[1\text{The series approximation to the expression } \frac{1}{b^2} \frac{e^{-2r/b}}{(1-e^{-r/b})^2} \approx \frac{1}{r^2} - \frac{1}{br}, \text{ it includes a Coulomb term.} \]
\[
\frac{1}{r^2} \approx \frac{1}{b^2 \left(1 - e^{-r/b}\right)^2}, \quad (13)
\]
in a short potential range. To solve it by the present method, we need to recast Eq. (12) with Eq. (13) into the form of Eq. (4) changing the variables \( r \rightarrow z \) through the mapping function \( r = f(z) \) and energy transformation given by
\[
z = e^{-r/b}, \quad \varepsilon = \sqrt{-\frac{2\mu b^2 E_{nl}}{\hbar^2}}, \quad E_{nl} < 0,
\]
(14)
to obtain the following hypergeometric equation:
\[
\frac{d^2 R(z)}{dz^2} + \frac{(1 - z) dR(z)}{z(1 - z)} dz + \frac{1}{\left[z(1 - z)\right]^2} \left\{ -\varepsilon^2 + [A + 2\varepsilon^2 - l(l + 1)] z - [A + \varepsilon^2 + \alpha(\alpha - 1)] z^2 \right\} R_{nl}(z) = 0.
\]
(15)
We notice that for bound state (real) solutions, the last equation requires that
\[
z = \begin{cases} 
0, & \text{when } r \rightarrow \infty, \\
1, & \text{when } r \rightarrow 0,
\end{cases}
\]
(16)
and thus the finite radial wavefunctions \( R_{nl}(z) \rightarrow 0 \). To apply the NU method, it is necessary to compare Eq. (15) with Eq. (4). Subsequently, the following value for the parameters in Eq. (4) are obtained as
\[
\tilde{\tau}(z) = 1 - z, \quad \sigma(z) = z - z^2, \quad \tilde{\sigma}(z) = -\left[A + \varepsilon^2 + \alpha(\alpha - 1)\right] z^2 + \left[A + 2\varepsilon^2 - l(l + 1)\right] z - \varepsilon^2.
\]
(17)
If one inserts these values of parameters into Eq. (9), with \( \sigma'(z) = 1 - 2z \), the following linear function is achieved
\[
\pi(z) = -\frac{z}{2} \pm \frac{1}{2} \sqrt{\left\{1 + 4 \left[A + \varepsilon^2 + \alpha(\alpha - 1)\right] - k\right\} z^2 + 4 \{k - [A + 2\varepsilon^2 - l(l + 1)]\} z + 4\varepsilon^2}.
\]
(18)
According to this method the expression in the square root has to be set equal to zero, that is, \( \Delta = \left\{1 + 4 \left[A + \varepsilon^2 + \alpha(\alpha - 1)\right] - k\right\} z^2 + 4 \{k - [A + 2\varepsilon^2 - l(l + 1)]\} z + 4\varepsilon^2 = 0 \). Thus the constant \( k \) can be determined as
\[ k = A - l(l + 1) \pm a\varepsilon, \quad a = \sqrt{(1 - 2\alpha)^2 + 4l(l + 1)}. \] (19)

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

\[
\pi(z) = -\frac{z}{2} \pm \begin{cases} 
\varepsilon - \left(\varepsilon - \frac{a}{2}\right)z, & \text{for} \quad k = A - l(l + 1) + a\varepsilon, \\
\varepsilon - \left(\varepsilon + \frac{a}{2}\right)z; & \text{for} \quad k = A - l(l + 1) - a\varepsilon.
\end{cases}
\] (20)

We must select

\[ k = A - l(l + 1) - a\varepsilon, \quad \pi(z) = -\frac{z}{2} + \varepsilon - \left(\varepsilon + \frac{a}{2}\right)z, \] (21)

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

\[
\tau(z) = 1 + 2\varepsilon - (2 + 2\varepsilon + a)z, \quad \tau'(z) = -(2 + 2\varepsilon + a). \] (22)

We can also write the values of \( \lambda = k + \pi'(z) \) and \( \lambda_n = -n\pi'(z) - \frac{n(n-1)}{2}\sigma''(z), \quad n = 0, 1, 2, ... \) as

\[
\lambda = A - l(l + 1) - (1 + a)\left[\frac{1}{2} + \varepsilon\right], \] (23)

\[
\lambda_n = n(1 + n + a + 2\varepsilon), \quad n = 0, 1, 2, ...
\] (24)

respectively. Additionally, using the definition of \( \lambda = \lambda_n \) and solving the resulting equation for \( \varepsilon \), allows one to obtain

\[
\varepsilon = \frac{(n + 1)^2 + l(l + 1) + (2n + 1)\Lambda - A}{2(n + 1 + \Lambda)}, \quad \Lambda = \frac{-1 + a}{2}, \] (25)

from which we obtain the discrete energy levels

\[
E_{nl} = -\frac{\hbar^2}{2\mu b^2} \left[\frac{(n + 1)^2 + l(l + 1) + (2n + 1)\Lambda - A}{2(n + 1 + \Lambda)}\right]^2, \quad 0 \leq n, l < \infty \] (26)

where \( n \) denotes the radial quantum number. It is found that \( \Lambda \) remains invariant by mapping \( \alpha \to 1 - \alpha \), so do the bound state energies \( E_{nl} \). An important quantity of interest for the Manning-Rosen 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. Using Eq. (26), in atomic units \( \hbar^2 = \mu = Z = e = 1 \),
\[ A_c = (n + 1 + \Lambda)^2 - \Lambda(\Lambda + 1) + l(l + 1). \] (27)

Let us now find the corresponding radial part of the wave function. Using \( \sigma(z) \) and \( \pi(z) \) in Eqs (17) and (21), we obtain

\[ \phi(z) = z^\varepsilon (1 - z)^{(\Lambda+1)/2}, \] (28)

\[ \rho(z) = z^{2\varepsilon} (1 - z)^{2\Lambda+1}, \] (29)

\[ y_{nl}(z) = C_n z^{-2\varepsilon} (1 - z)^{-(2\Lambda+1)} \frac{d^n}{dz^n} \left[ z^{n+2\varepsilon} (1 - z)^{n+2\Lambda+1} \right]. \] (30)

The functions \( y_{nl}(z) \) are, up to a numerical factor, are in the form of Jacobi polynomials, i.e., \( y_{nl}(z) \sim P_n^{(2\varepsilon,2\Lambda+1)}(1 - 2z) \), valid physically in the interval \( 0 \leq r < \infty \rightarrow 0 \leq z \leq 1 \) [54]. Therefore, the radial part of the wave functions can be found by substituting Eqs. (28) and (30) into \( R_{nl}(z) = \phi(z) y_{nl}(z) \) as

\[ R_{nl}(z) = N_{nl} z^\varepsilon (1 - z)^{1+\Lambda} P_n^{(2\varepsilon,2\Lambda+1)}(1 - 2z), \] (31)

where \( \varepsilon \) and \( \Lambda \) are given in Eqs. (14) and (19) and \( N_{nl} \) is a normalization constant. This equation satisfies the requirements; \( R_{nl}(z) = 0 \) as \( z = 0 \) (\( r \rightarrow \infty \)) and \( R_{nl}(z) = 0 \) as \( z = 1 \) (\( r = 0 \)). Therefore, the wave functions, \( R_{nl}(z) \) in Eq. (31) is valid physically in the closed interval \( z \in [0, 1] \) or \( r \in (0, \infty) \). Further, the wave functions satisfy the normalization condition

\[ \int_0^\infty |R_{nl}(r)|^2 dr = 1 = b \int_0^1 z^{-1} |R_{nl}(z)|^2 dz, \] (32)

where \( N_{nl} \) can be determined via

\[ 1 = b N_{nl}^2 \int_0^1 z^{2\varepsilon-1} (1 - z)^{2\Lambda+2} \left[ P_n^{(2\varepsilon,2\Lambda+1)}(1 - 2z) \right]^2 dz. \] (33)

The Jacobi polynomials, \( P_n^{(\rho,\nu)}(\xi) \), can be explicitly written in two different ways [55,56]:

\[ P_n^{(\rho,\nu)}(\xi) = 2^{-n} \sum_{p=0}^n (-1)^{n-p} \binom{n+\rho}{p} \binom{n+\nu}{n-p} (1 - \xi)^{n-p} (1 + \xi)^p, \] (34)
\[ P_{n}^{(\rho,\nu)}(\xi) = \frac{\Gamma(n + \rho + 1)}{n!\Gamma(n + \rho + \nu + 1)} \sum_{r=0}^{n} \binom{n}{r} \frac{\Gamma(n + \rho + \nu + r + 1)}{\Gamma(r + \rho + 1)} \left(\frac{\xi - 1}{2}\right)^{r}, \quad(35) \]

where \( \binom{n}{r} = \frac{n!}{r!(n-r)!} = \frac{\Gamma(n+1)}{\Gamma(r+1)\Gamma(n-r+1)} \). Using Eqs. (34)-(35), we obtain the explicit expressions for \( P_{n}^{(2\varepsilon,2\Lambda+1)}(1-2z) \):

\[ P_{n}^{(2\varepsilon,2\Lambda+1)}(1-2z) = (-1)^{n}\Gamma(n + 2\varepsilon + 1)\Gamma(n + 2\Lambda + 2) \times \sum_{p=0}^{n} \frac{(-1)^{p}}{p!(n-p)!\Gamma(p + 2\Lambda + 2)\Gamma(n + 2\varepsilon - p + 1)} z^{n-p}(1 - z)^{p}, \quad(36) \]

\[ P_{n}^{(2\varepsilon,2\Lambda+1)}(1-2z) = \frac{\Gamma(n + 2\varepsilon + 1)}{\Gamma(n + 2\varepsilon + 2\Lambda + 2)} \sum_{r=0}^{n} \frac{(-1)^{r}\Gamma(n + 2\varepsilon + 2\Lambda + r + 2)}{r!(n-r)!\Gamma(2\varepsilon + r + 1)} z^{r}. \quad(37) \]

Inserting Eqs. (36)-(37) into Eq. (33), one obtains

\[ 1 = bN_{n0}^{2}(1) = \frac{(-1)^{n}}{\Gamma(n + 2\Lambda + 2)\Gamma(n + 2\varepsilon + 1)^{2}} \times \sum_{p,r=0}^{n} \frac{(-1)^{p+r}\Gamma(n + 2\varepsilon + 2\Lambda + r + 2)}{p!(n-p)!(n-r)!\Gamma(p + 2\Lambda + 2)\Gamma(n + 2\varepsilon - p + 1)\Gamma(2\varepsilon + r + 1)} I_{n0}(p, r), \quad(38) \]

where

\[ I_{n0}(p, r) = \int_{0}^{1} z^{n+2\varepsilon+r-p-1}(1 - z)^{p+2\Lambda+2}dz. \quad(39) \]

Using the following integral representation of the hypergeometric function [55.56]

\[ _{2}F_{1}(\alpha_{0}, \beta_{0} : \gamma_{0}; 1) \frac{\Gamma(\alpha_{0})\Gamma(\gamma_{0} - \alpha_{0})}{\Gamma(\gamma_{0})} = \int_{0}^{1} z^{\alpha_{0}-1}(1 - z)^{\gamma_{0}-\alpha_{0}-1}(1 - z)^{-\beta_{0}}dz, \quad(40) \]

\[ \text{Re}(\gamma_{0}) > \text{Re}(\alpha_{0}) > 0, \]

which gives

\[ _{2}F_{1}(\alpha_{0}, \beta_{0} : \alpha_{0} + 1; 1) = \frac{1}{\alpha_{0}} \int_{0}^{1} z^{\alpha_{0}-1}(1 - z)^{-\beta_{0}}dz, \quad(41) \]

where

9
\[ 2F_1(\alpha_0, \beta_0 : \gamma_0; 1) = \frac{\Gamma(\gamma_0)\Gamma(\gamma_0 - \alpha_0 - \beta_0)}{\Gamma(\gamma_0 - \alpha_0)\Gamma(\gamma_0 - \beta_0)}, \]

\[ (\text{Re}(\gamma_0 - \alpha_0 - \beta_0) > 0, \text{Re}(\gamma_0) > \text{Re}(\beta_0) > 0). \] (42)

For the present case, with the aid of Eq. (40), when \( \alpha_0 = n + 2\varepsilon + r - p, \beta_0 = -p - 2\Lambda - 2, \) and \( \gamma_0 = \alpha_0 + 1 \) are substituted into Eq. (41), we obtain

\[ I_{nl}(p, r) = \frac{2F_1(\alpha_0, \beta_0 : \gamma_0; 1)}{\alpha_0} = \frac{\Gamma(n + 2\varepsilon + r - p + 1)\Gamma(p + 2\Lambda + 3)}{(n + 2\varepsilon + r - p)\Gamma(n + 2\varepsilon + r + 2\Lambda + 3)}. \] (43)

Finally, we obtain

\[ 1 = bN_{nl}^2(-1)^n\frac{\Gamma(n + 2\Lambda + 2)\Gamma(n + 2\varepsilon + 1)^2}{\Gamma(n + 2\varepsilon + 2\Lambda + 2)} \times \sum_{p, r = 0}^{n} (-1)^{p+r}\frac{\Gamma(n + 2\varepsilon + r - p + 1)(p + 2\Lambda + 2)}{(n - p)!(n - r)!\Gamma(n + 2\varepsilon - p + 1)\Gamma(2\varepsilon + r + 1)(n + 2\varepsilon + r + 2\Lambda + 2)}, \] (44)

which gives

\[ N_{nl} = \frac{1}{\sqrt{s(n)}}, \] (45)

where

\[ s(n) = b(-1)^n\frac{\Gamma(n + 2\Lambda + 2)\Gamma(n + 2\varepsilon + 1)^2}{\Gamma(n + 2\varepsilon + 2\Lambda + 2)} \times \sum_{p, r = 0}^{n} (-1)^{p+r}\frac{\Gamma(n + 2\varepsilon + r - p + 1)(p + 2\Lambda + 2)}{(n - p)!(n - r)!\Gamma(n + 2\varepsilon - p + 1)\Gamma(2\varepsilon + r + 1)(n + 2\varepsilon + r + 2\Lambda + 2)}. \] (46)

**IV. 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 \( \alpha \). Its shown in Table 1, the present approximately numerical results are not in a good agreement when long potential range (small values of parameter \( b \)). 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.
V. DISCUSSIONS

In this work, we have utilized NU method and solved the radial SE for the Manning-Rosen model potential with the angular momentum \( l \neq 0 \) states. We have derived the binding energy spectra in Eq. (26) and their corresponding wave functions in Eq. (31).

Let us study special cases. We have shown that for \( \alpha = 0 \) (1), the present solution reduces to the one of the Hulthén potential [16,18,19]:

\[
V^{(H)}(r) = -V_0 \frac{e^{-\delta r}}{1 - e^{-\delta r}}, \quad V_0 = Ze^2\delta, \quad \delta = b^{-1} \tag{47}
\]

where \( Ze^2 \) is the strength and \( \delta \) is the screening parameter and \( b \) is the range of potential. 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

\[
E_{nl} = - \left[ \frac{A - (n + l + 1)^2}{8\mu b^2(n + l + 1)^2} \right], \quad 0 \leq n, l < \infty. \tag{48}
\]

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

\[
E_n = - \left[ \frac{A - (n + 1)^2}{8\mu b^2(n + 1)^2} \right], \quad 0 \leq n < \infty \tag{49}
\]

Essentially, these results coincide with those obtained by the Feynman integral method [31] and the standard way [32,33], respectively. Furthermore, in taking \( b = 1/\delta \) and identifying \( \frac{\Delta b^2}{2\mu b^2} \) as \( Ze^2\delta \), we are able to obtain

\[
E_{nl} = - \frac{\mu (Ze^2)^2}{2\hbar^2} \left[ \frac{1}{n + l + 1} - \frac{\hbar^2 \delta}{2Ze^2\mu}(n + l + 1) \right]^2, \tag{50}
\]

which coincides with those of Refs. [16,18]. With natural units \( \hbar^2 = \mu = Z = e = 1 \), we have

\[
E_{nl} = - \frac{1}{2} \left[ \frac{1}{n + l + 1} - \frac{(n + l + 1)}{2} \delta \right]^2, \tag{51}
\]

which coincides with Refs. [16,33].

The corresponding radial wave functions are expressed as
\[ R_{nl}(r) = N_{nl}e^{-\delta r}(1 - e^{-\delta r})^{l+1}P_n^{(2l,2l+1)}(1 - 2e^{-\delta r}), \]

where

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

which coincides for the ground state with that given in Eq. (6) by Gönül et al [18]. 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 wavefunctions:

\[ E_{nl} = -\frac{\varepsilon_0}{(n + l + 1)^2}, \quad n = 0, 1, 2, \ldots \]

\[ \varepsilon_0 = \frac{Z^2 \hbar^2}{2\mu a_0^2}, \quad a_0 = \frac{\hbar^2}{\mu e^2} \]

where \( \varepsilon_0 = 13.6 \) eV and \( a_0 \) is Bohr radius for the Hydrogen atom. The wave functions are

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

which coincide with Refs. [3,16,22].

**VI. CONCLUDING REMARKS**

In this work, we have presented the approximate solutions of the \( l \)-wave Schrödinger equation with the Manning-Rosen potential. The special cases for \( \alpha = 0, 1 \) are discussed. The results are in good agreement with those obtained by other methods for short potential range, small \( \alpha \) 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 constitute a reliable alternative way in solving the exponential potentials.

**ACKNOWLEDGMENTS**

This research was partially supported by the Scientific and Technological Research Council of Turkey.
REFERENCES

[1] L.I. Schiff, Quantum Mechanics 3rd edn. (McGraw-Hill Book Co., New York, 1968).

[2] L.D. Landau and E.M. Lifshitz, Quantum Mechanics, Non-relativistic Theory, 3rd edn. (Pergamon, New York, 1977).

[3] M.M. Neito, Am. J. Phys. 47 (1979) 1067.

[4] Ş. Erkoç and R. Sever, Phys. Rev. D 30 (1984) 2117; D 33 (1986) 588; Phys. Rev. A 37 (1988) 2687.

[5] M.L. Sage, Chem. Phys. 87 (1984) 431; M. Sage and J. Goodisman, Am. J. Phys. 53 (1985) 350.

[6] S.-H. Dong, Appl. Math. Lett. 16 (2003) 199.

[7] S. Ikhdair and R. Sever, J. Mol. Struct.-Theochem 806 (2007) 155.

[8] S.M. Ikhdair and R. Sever, preprint quant-ph/0611065, to appear in J. Mol. Struct.-Theochem (2008).

[9] C.L. Pekeris, Phys. Rev. 45 (1934) 98.

[10] C. Berkdemir, Nucl. Phys. A 770 (2006) 32.

[11] W.-C. Qiang and S.-H. Dong, Phys. Lett. A 363 (2007) 169.

[12] C. Berkdemir and J. Han, Chem. Phys. Lett. 409 (2005) 203.

[13] W.-C. Qiang and S.-H. Dong, Phys. Lett. A 363 (2007) 169.

[14] C. Berkdemir, A. Berkdemir and J. Han, Chem. Phys. Lett. 417 (2006) 326.

[15] P.M. Morse, Phys. Rev. 34 (1929) 57.

[16] S.M. Ikhdair and R. Sever, J. Math. Chem. 42 (3) (2007) 461.

[17] M. Şimşek and H. Eğrifes, J. Phys. A: Math. Gen. 37 (2004) 4379.
[18] B. Göñül and İ. Zorba, Phys. Lett. A 269 (2000) 83; R.L. Greene and C. Aldrich, Phys. Rev. A 14 (1976) 2363.

[19] L. Hulthén, Ark. Mat. Astron. Fys. A 28 (1942) 5.

[20] Ö. Yeşiltaş, Phys. Scr. 75 (2007) 41.

[21] S.M. Ikhdair and R. Sever, Ann. Phys. (Berlin) 16 (2007) 218.

[22] S.M. Ikhdair and R. Sever, Int. J. Theor. Phys. 46 (6) (2007) 1643.

[23] S.M. Ikhdair and R. Sever, preprint quant-ph/0605045, to appear in the Int. J. Mod. Phys. E.

[24] C. Berkdemir, Am. J. Phys. 75 (2007) 81.

[25] Y.-F. Cheng and T.-Q. Dai, Phys. Scr. 75 (2007) 274; Chinese J. Phys. 45 (5) (2007) 480.

[26] S.M. Ikhdair and R. Sever, Int. J. Mod. Phys. C 18 (10) (2007) 1571; Centr. Eur. J. Phys. 5 (4) (2007) 516; preprint quant-ph/0702052 to appear in the Centr. Eur. J. Phys.; S.M. Ikhdair, preprint quant-ph/0703042, to appear in the Chinese J. Phys.

[27] W.-C. Qiang, Chin. Phys. 12 (2003) 1054; 13 (2004) 575.

[28] L.-Z. Yi, Y.-F. Diao, J.-Y. Liu and C.-S. Jia, Phys. Lett. A 333 (2004) 212.

[29] N. Rosen and P.M. Morse, Phys. Rev. 42 (1932) 210.

[30] M.F. Manning, Phys. Rev. 44 (1933) 951; M.F. Manning and N. Rosen, Phys. Rev. 43 (1933) 671.

[31] A. Diaf, A. Chouchaoui and R.L. Lombard, Ann. Phys. (Paris) 317 (2005) 354.

[32] S.-H. Dong and J. Garcia-Ravelo, Phys. Scr. 75 (2007) 307.

[33] W.-C. Qiang and S. H. Dong, Phys. Lett. A 368 (2007) 13.
[34] C.-S. Jia et al., J. Phys. A: Math. Gen. 37 (2004) 11275; C.-S. Jia et al., Phys. Lett. A 311 (2003) 115.

[35] H. Eğrifes, D. Demirhan and F. Büyükkılıç, Phys. Lett. A 275 (2000) 229.

[36] D.A. Morales, Chem. Phys. Lett. 394 (2004) 68.

[37] E.D. Filho and R.M. Ricotta, Phys. Lett. A 269 (2000) 269.

[38] O. Bayrak, I. Boztosun and H. Çiftçi, Int. J. Quantum Chem. 107 (2007) 540; O. Bayrak and I. Boztosun, J. Phys. A: Math. Gen. 39 (2006) 6955.

[39] Z.-Q. Ma and B.-W. Xu, Europhys. Lett. 69 (2005) 685.

[40] S.-H. Dong, D. Morales and J. Garcia-Ravelo, Int. J. Mod. Phys. E 16 (2007) 189.

[41] J.P. Killingbeck, A. Grosjean and G. Jolicard, J. Chem. Phys. 116 (2002) 447.

[42] S.M. Ikhdair and R. Sever, Z. Phys. C 56 (1992) 155; C 58 (1993) 153; D 28 (1993) 1; Hadronic J. 15 (1992) 389; Int. J. Mod. Phys. A 18 (2003) 4215; A 19 (2004) 1771; A 20 (2005) 4035; A 20 (2005) 6509; A 21 (2006) 2191; A 21 (2006) 3989; A 21 (2006) 6699; Int. J. Mod. Phys. E (in press) (preprint hep-ph/0504176); S. Ikhdair et al, Tr. J. Phys. 16 (1992) 510; 17 (1993) 474.

[43] M. Bag, M.M. Panja and R. Dutt, Phys. Rev. A 46 (1992) 6059.

[44] J.Yu, S.-H. Dong and G.H. Sun, Phys. Lett. A 322 (2004) 290.

[45] R.L. Hall and N. Saad, J. Chem. Phys. 109 (1998) 2983.

[46] M.R. Setare and E. Karimi, Phys. Scr. 75 (2007) 90.

[47] B. Gönül, Chin. Phys. Lett. 21 (2004) 1685; 21 (2004) 2330; B. Gönül, K. Köksal and E. Bakır, Phys. Scr. 73 (2006) 279.

[48] S.M. Ikhdair and R. Sever, J. Math. Chem 41 (2007) 329; 41 (2007) 343; J. Molec. Struc. (Theochem) 809 (2007) 103; Int. J. Mod. Phys. A 21 (2006) 6465.
[49] S.M. Ikhdair and R. Sever, Int. J. Theor. Phys. 46 (10) (2007) 2384.

[50] C. Berkdemir, A. Berkdemir and R. Sever, J. Phys. A: Math. Gen. 39 (2006) 13455.

[51] A.F. Nikiforov and V.B. Uvarov, Special Functions of Mathematical Physics (Birkhauser, Bassel, 1988).

[52] R.J. Le Roy and R.B. Bernstein, J. Chem. Phys. 52 (1970) 3869.

[53] J. Cai, P. Cai and A. Inomata, Phys. Rev. A 34 (1986) 4621.

[54] M. Abramowitz and I.A. Stegun, Handbook of Mathematical Functions (Dover, New York, 1964).

[55] G. Sezgo, Orthogonal Polynomials (American Mathematical Society, New York, 1939).

[56] N.N. Lebedev, Special Functions and Their Applications (Prentice-Hall, Englewood Cliffs, NJ, 1965).

[57] W. Lucha and F.F. Schöberl, Int. J. Mod. Phys. C 10 (1999) 607.
TABLE I. Eigenvalues for 2p, 3p, 3d, 4p, 4d, 4f, 5p, 5d, 5f, 5g, 6p, 6d, 6f and 6g states in atomic units ($\hbar = \mu = 1$) and for $\alpha = 0.75$ and $\alpha = 1.5$, $A = 2b$.

| states | $1/b$ | present | QD [33] | LS [57] | present | QD [33] | LS [57] |
|--------|-------|---------|---------|---------|---------|---------|---------|
| 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 | −0.010947 | −0.010947 | −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 |
TABLE II. Energy levels of HCl and CH (in eV) for 2p, 3p, 3d, 4p, 4d, 4f, 5p, 5d, 5f, 5g, 6p, 6d, 6f and 6g states where \( hc = 1973.29 \) eV \( A^\circ \), \( \mu_{HCl} = 0.9801045 \) amu, \( \mu_{CH} = 0.929931 \) 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   | -1.10712478    | -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    | -0.82535374    |
|        | 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 |

\(^a_\text{b is in pm.}\)
TABLE III. Energy levels of \( LiH \) and \( CO \) (in eV) for \( 2p, 3p, 3d, 4p, 4d, 4f, 5p, 5d, 5f, 5g, 6p, 6d, 6f \) and \( 6g \) states where \( \hbar c = 1973.29 \) eV \( A^0 \), \( \mu_{LiH} = 0.8801221 \) amu, \( \mu_{CO} = 6.8606719 \) amu and \( A = 2b \).

| states \( 1/b^a \) | \( LiH/ \alpha = 0 \) | \( \alpha = 0.75 \) | \( \alpha = 1.5 \) | \( CO/ \alpha = 0 \) | \( \alpha = 0.75 \) | \( \alpha = 1.5 \) |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| \( 2p \)        | 0.025 \(-5.35811876\) | \(-5.7270906\) | \(-4.27570397\) | \(-1.374733789\) | \(-0.734690030\) | \(-0.548509185\) |
|                 | 0.050 \(-4.80894870\) | \(-5.14962650\) | \(-3.81140413\) | \(-1.233833096\) | \(-0.660620439\) | \(-0.488946426\) |
|                 | 0.075 \(-4.28946350\) | \(-4.60291196\) | \(-3.37377992\) | \(-1.100548657\) | \(-0.590485101\) | \(-0.432805497\) |
|                 | 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 |

\(^{ab}\) is in pm.