

On the bound-state solutions of the Manning-Rosen potential including improved approximation to the orbital centrifugal term

Sameer M. Ikhdaïr^{1,*}

¹*Physics Department, Near East University, Nicosia, Mersin 10, Turkey*

(Dated: April 5, 2011)

Abstract

The approximate analytical bound state solution of the Schrödinger equation for the Manning-Rosen potential is carried out by taking a new approximation scheme to the orbital centrifugal term. The Nikiforov-Uvarov method is used in the calculations. We obtain analytic forms for the energy eigenvalues and the corresponding normalized wave functions in terms of the Jacobi polynomials or hypergeometric functions for different screening parameters $1/b$. The rotational-vibrational energy states for a few diatomic molecules are calculated for arbitrary quantum numbers n and l with different values of the potential parameter α . The present numerical results agree within five decimal digits with the previously reported results for different $1/b$ values. A few special cases of the s -wave ($l = 0$) Manning-Rosen potential and the Hulthén potential are also studied.

Keywords: Energy eigenvalues; Manning-Rosen potential; Nikiforov-Uvarov method, Approximation schemes.

PACS numbers: 03.65.-w; 02.30.Gp; 03.65.Ge; 34.20.Cf

*E-mail: sikhdaïr@neu.edu.tr

I. INTRODUCTION

The exact analytic solutions of the wave equations (nonrelativistic and relativistic) are only possible for certain potentials of physical interest under consideration since they contain all the necessary information on the quantum system. 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, the pseudoharmonic potentials and others [1-5]. The analytic exact solutions of the wave equation with some exponential-type potentials are impossible for $l \neq 0$ states. Therefore, approximation schemes have to be used to deal with the orbital centrifugal term like the Pekeris approximation [6-8] and the approximated scheme suggested by Greene and Aldrich [9]. Some of these exponential-type potentials include the Morse potential [10], the Hulthén potential [11], the Pöschl-Teller [12], the Woods-Saxon potential [13], the Kratzer-type and pseudoharmonic potentials [14], the Rosen-Morse-type potentials [15], the Manning-Rosen potential [16-19] and other multiparameter exponential-type potentials [20,21] etc.

The Manning-Rosen (MR) potential has been one of the most useful and convenient models to study the energy eigenvalues of diatomic molecules [16]. As an empirical potential, the MR potential gives an excellent description of the interaction between the two atoms in a diatomic molecule and also it is very reasonable in describing such interactions close to the surface. The short range MR potential is defined by [16-19]

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

where A and α are two constants and the parameter b characterizes the range of the potential [22]. The above potential may be further put in the following simple form

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

which is usually used for the description of diatomic molecular vibrations and rotations [23,24]. It is also used in several branches of physics for their bound states and scattering properties. This potential remains invariant by mapping $\alpha \rightarrow 1 - \alpha$ and has a relative minimum at $r_0 = b \ln [1 + 2\alpha(\alpha - 1)/A]$ with value $V(r_0) = -\frac{\hbar^2 A^2}{8\mu b^2 \alpha(\alpha - 1)}$ for $\alpha < 0$ or $\alpha > 1$ and $A > 0$. Moreover, the second derivative determines the force constants at $r = r_0$ which

is given by

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

If $\alpha = 0$ or $\alpha = 1$, the potential (1) reduces to the Hulthén potential [11]. For the potential in Eq. (1) [16-19], the Schrödinger equation (SE) can be easily solved for the s -wave, angular momentum quantum number $l = 0$. However, for the general solution, one needs to include some approximations to obtain analytical or semi-analytical solutions to the SE. Also, it is often necessary to determine the l -wave ($l \neq 0$ states), so an analytic procedure would be advantageous [25-27]. Hence, in the previous papers, several approximations have been developed to find better analytical formulas for the energy bound states and wave functions. For instance, in the $l = 0$ case, the bound-state energy spectra for the MR potential have already been calculated by using the path-integral approach [17] and function analysis method [18]. For the $l \neq 0$ case, the potential can not be solved exactly without using approximation scheme. Recently, Qiang and Dong [19] approximated the centrifugal term

$$\frac{1}{r^2} \approx \frac{1}{b^2} \left[\frac{1}{e^{r/b} - 1} + \frac{1}{(e^{r/b} - 1)^2} \right] = \frac{1}{b^2} \frac{e^{r/b}}{(e^{r/b} - 1)^2}$$

and studied l -wave bound-state solutions of the SE for MR potential. Further, the scattering state solutions for the same potential and approximation have also been investigated [25]. The above approximation has also been applied to obtain the l -wave solutions of SE with the MR potential in three-dimensions and D -dimensions and also with the Hulthén potential using the Nikiforov and Uvarov (NU) method [11,19,26,27]. The present approximations provide good results which are in agreement within five decimal digits with the previously reported numerical integration method by Lucha and Schöberl [28] for short-range potential (large b and small l) but not for long-range potential (small b and large l).

The main purpose of the present paper is to improve the accuracy of the previous approximations introduced in [26,29], so that we apply a different approximation scheme recently proposed in Ref. [27] for the centrifugal term $l(l+1)r^{-2}$ to make the results in higher agreement with Ref. [28]. Thus, with this new approximation scheme, we calculate the $l \neq 0$ energy levels and wave functions for the MR potential using the NU method [30] which has shown its power in calculating the exact energy levels for some solvable quantum systems. For this, the results are in better agreement with those obtained by means of numerical

integration method [28]. As an illustration, the method is applied to find the ro-vibrational energy states for a few diatomic molecules: HCl, CH, LiH, CO, NO, O₂, I₂, N₂, H₂ and Ar₂.

The paper is organized as follows: In Section II, we apply the new approximation scheme to calculate the l -wave bound state eigensolutions of the SE for MR potential by using the NU method. In Section III, we present our ro-vibrational energy levels for a few diatomic molecules. Section IV, is devoted for two special cases, namely, s -wave ($l = 0$) and the Hulthén potential. Finally, we make a few concluding remarks in Section V.

II. BOUND STATE SOLUTIONS

To study any quantum physical system, we solve the original SE that is given in the well known textbooks [1,2]

$$\left(\frac{p^2}{2m} + V(r)\right)\psi_{nlm}(\mathbf{r}) = E_{nl}\psi_{nlm}(\mathbf{r}), \quad (4)$$

where the potential $V(r)$ is taken as the MR form in (1). Further, we set the wave functions $\psi_{nlm}(\mathbf{r}) = \frac{u_{nl}(r)}{r}Y_{lm}(\theta, \phi)$ to obtain the following radial Schrödinger equation:

$$\frac{d^2u_{nl}(r)}{dr^2} + \left[\frac{2\mu E_{nl}}{\hbar^2} - V_{\text{eff}}(r)\right]u_{nl}(r) = 0, \quad (5a)$$

$$V_{\text{eff}}(r) = \frac{1}{b^2} \left[\frac{\alpha(\alpha - 1)}{(e^{r/b} - 1)^2} - \frac{A}{e^{r/b} - 1} \right] + \frac{l(l + 1)}{r^2}, \quad (5b)$$

in which $u_{nl}(0) = 0$ and $\lim_{r \rightarrow \infty} u_{nl}(r) = 0$. To solve the above equation for $l \neq 0$ states, we need to apply the following approximate scheme to the centrifugal term given by

$$\frac{1}{r^2} \approx \frac{1}{b^2} \left[D_0 + D_1 \frac{1}{e^{r/b} - 1} + D_2 \frac{1}{(e^{r/b} - 1)^2} \right], \quad (6)$$

and the higher order terms are neglected. These solutions are valid for $r/b \ll 1$, that is, the solutions obtained are valid for $\alpha(\alpha - 1)/A \ll 1$ but positive. Obviously, the above approximation to the centrifugal term turns to r^{-2} when the parameter b goes to infinity (small screening parameter $\delta = 1/b$) as

$$\lim_{b \rightarrow \infty} \left[\frac{1}{b^2} \left(D_0 + \frac{1}{e^{r/b} - 1} + \frac{1}{(e^{r/b} - 1)^2} \right) \right] = \frac{1}{r^2}, \quad (6a)$$

which shows that the usual approximation is the limit of our approximation (cf. e.g., [31] and the references therein). The values of the parameters D_i ($i = 0, 1$ and 2) are given by

[27,31]

$$D_0 \simeq \frac{1}{12}, \quad D_1 = D_2 = 1. \quad (7)$$

However, the values of the parameters D_i ($i = 0, 1$ and 2) used by Wei and Dong [32] are given by

$$D_0 = \frac{12\epsilon_1^2 - 4\epsilon_1(2A + 3\epsilon_1)\log(\epsilon_2) + \epsilon_3^2\log(\epsilon_2)^2}{\epsilon_4^2\log(\epsilon_2)^4}, \quad (8a)$$

$$D_1 = \frac{8\epsilon_1^2[-6\epsilon_1 + (3A + 4\epsilon_1)\log(\epsilon_2)]}{A\epsilon_4^2\log(\epsilon_2)^4}, \quad (8b)$$

$$D_2 = -\frac{16\epsilon_1^3[-3\epsilon_1 + \epsilon_3\log(\epsilon_2)]}{A^2\epsilon_4^2\log(\epsilon_2)^4}, \quad (8c)$$

where $\epsilon_1 = \alpha(\alpha - 1)$, $\epsilon_2 = 1 + 2\alpha(\alpha - 1)/A$, $\epsilon_3 = A\epsilon_2$ and $\epsilon_4 = b\epsilon_3$.

Now, we need to recast differential equation (5) and the approximation (6) into the form of Eq. (1) of Ref. [33] by introducing the change in the variables $r \rightarrow z$ through the mapping function $z = e^{-r/b}$, and defining

$$\varepsilon_{nl} = \sqrt{-\frac{2\mu b^2 E_{nl}}{\hbar^2} + \Delta E_l} > 0, \quad E_{nl} < \frac{\hbar^2}{2\mu b^2} \Delta E_l, \quad \Delta E_l = l(l+1)D_0, \quad (9a)$$

$$\beta_1 = A - l(l+1)D_1, \quad (9b)$$

$$\beta_2 = \alpha(\alpha - 1) + l(l+1)D_2, \quad (9c)$$

in order to obtain the following compact hypergeometric equation:

$$\begin{aligned} & \frac{d^2 u_{nl}(z)}{dz^2} + \frac{(1-z)}{z(1-z)} \frac{du_{nl}(z)}{dz} \\ & + \frac{1}{[z(1-z)]^2} \{-\varepsilon_{nl}^2 + (2\varepsilon_{nl}^2 + \beta_1)z - (\varepsilon_{nl}^2 + \beta_1 + \beta_2)z^2\} u_{nl}(z) = 0. \end{aligned} \quad (10)$$

We notice that for the presence of bound state (real) solutions, ε_{nl} must be a positive real parameter and we require that

$$z = \begin{cases} 0, & \text{when } r \rightarrow \infty, \\ 1, & \text{when } r \rightarrow 0, \end{cases} \quad (11)$$

for the radial wave functions to fulfill the boundary conditions, i.e., $u_{nl}(0) \rightarrow 0$ and $u_{nl}(1) \rightarrow 0$. Let us begin by comparing Eq. (10) with Eq. (1) of Ref. [33], then we obtain the following definitions:

$$\tilde{\tau}(z) = 1 - z, \quad \sigma(z) = z - z^2, \quad \tilde{\sigma}(z) = -\varepsilon_{nl}^2 + (2\varepsilon_{nl}^2 + \beta_1)z - (\varepsilon_{nl}^2 + \beta_1 + \beta_2)z^2. \quad (12)$$

After applying the relations (A1-A4) of Ref. [33], the following useful functions usually defined by the NU method [30] are achieved

$$k = \beta_1 - a\varepsilon_{nl}, \quad a = \sqrt{(1 - 2\alpha)^2 + 4l(l + 1)D_2}. \quad (13)$$

$$\pi(z) = -\frac{z}{2} - \frac{1}{2}[(a + 2\varepsilon_{nl})z - a], \quad (14)$$

and

$$\tau(z) = 1 + 2\varepsilon_{nl} - (2 + 2\varepsilon_{nl} + a)z, \quad \tau'(z) = -(2 + 2\varepsilon_{nl} + a). \quad (15)$$

We can also write the values of $\lambda = k + \pi'(z)$ and $\lambda_n = -n\tau'(z) - \frac{n(n-1)}{2}\sigma''(z)$, $n = 0, 1, 2, \dots$ to obtain

$$\lambda = \beta_1 - (1 + a) \left(\frac{1}{2} + \varepsilon_{nl} \right), \quad (16)$$

and

$$\lambda_n = n(1 + n + a + 2\varepsilon_{nl}), \quad n = 0, 1, 2, \dots, \quad (17)$$

respectively. Furthermore, using the relation, $\lambda = \lambda_n$, or alternatively the energy equation (A5) of Ref. [33], allows one to obtain

$$\varepsilon_{nl} = \frac{A + \alpha(\alpha - 1) + l(l + 1)(D_2 - D_1)}{2n + 1 + a} - \frac{2n + 1 + a}{4}. \quad (18)$$

Plugging the parameters given in Eq. (9) into Eq. (18), we finally obtain the following discrete bound-state energy eigenvalues:

$$E_{nl} = E_{nl}^{(\text{approx})} = \frac{\hbar^2 l(l + 1)D_0}{2\mu b^2} - \frac{\hbar^2}{2\mu b^2} \left[\frac{A + \alpha(\alpha - 1) + l(l + 1)(D_2 - D_1)}{2n + 1 + \sqrt{(1 - 2\alpha)^2 + 4l(l + 1)D_2}} - \frac{2n + 1 + \sqrt{(1 - 2\alpha)^2 + 4l(l + 1)D_2}}{4} \right]^2, \quad (19)$$

where $0 \leq n \leq n_{\max}$ and $l = 0, 1, 2, \dots$, signify the usual vibrational and rotational quantum numbers, respectively. It is found that the parameter a in Eq. (13) remains invariant by mapping $\alpha \rightarrow 1 - \alpha$, 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. Hence, using Eq. (19), in atomic units $\hbar^2 = \mu = Z = e = 1$, we find the following critical coupling constant

$$A_c = \frac{1}{4} \left(2n + 1 + \sqrt{(1 - 2\alpha)^2 + 4l(l + 1)D_2} \right)^2 - \alpha(\alpha - 1) - l(l + 1)(D_2 - D_1). \quad (20)$$

Let us now turn to the calculations of the radial part of the normalized wave functions. After applying the relations (A6-A10) of Ref. [33], we obtain

$$\phi(z) = z^{\varepsilon_{nl}}(1-z)^{(1+a)/2}, \quad (21)$$

$$\rho(z) = z^{2\varepsilon_{nl}}(1-z)^a, \quad (22)$$

$$y_{nl}(z) = C_n z^{-2\varepsilon_{nl}}(1-z)^{-a} \frac{d^n}{dz^n} [z^{n+2\varepsilon_{nl}}(1-z)^{n+a}]. \quad (23)$$

The functions $y_{nl}(z)$, up to a numerical factor, are in the form of Jacobi polynomials, i.e., $y_{nl}(z) \simeq P_n^{(2\varepsilon_{nl}, a)}(1-2z)$ (the physical interval $(0, \infty)$ for variable r is mapped to the interval $(0, 1)$ for variable z) [13,14]. Hence, the approximated radial wave functions satisfying Eq. (5) are given by

$$u_{nl}(r) = u_{nl}^{(\text{approx})}(r) = \mathcal{N}_{nl} e^{-\varepsilon_{nl}r/b} (1 - e^{-r/b})^{\nu_l} {}_2F_1(-n, n + 2(\varepsilon_{nl} + \nu_l); 2\varepsilon_{nl} + 1; e^{-r/b}),$$

$$\varepsilon_{nl} > 0, \quad \nu_l = (1 + a) / 2 \geq 1, \quad (24)$$

where a and ε_{nl} are given in Eqs. (13) and (18), respectively and \mathcal{N}_{nl} is a normalization constant determined in the Appendix B.

When $l = 0$, we deal with s -wave case, the possible energies for the bound states and the corresponding wave functions are written explicitly, for $\alpha < 1/2$:

$$\left\{ \begin{array}{l} E_n = -\frac{\hbar^2}{8\mu b^2} \left[\frac{A+\alpha(\alpha-1)}{n-\alpha+1} - (n-\alpha+1) \right]^2; \\ n = 0, 1, 2, \dots, n_{\max} = \left[\sqrt{A + \alpha(\alpha-1)} + \alpha - 1 \right] \text{ and} \\ u_{n0}(r) = \mathcal{N}_n e^{-(\varepsilon_n/b)r} (1 - e^{-r/b})^{(1-\alpha)} \\ {}_2F_1(-n, n + 2(\varepsilon_n - \alpha + 1); 2\varepsilon_n + 1; e^{-r/b}), \end{array} \right. \quad (25)$$

where $\varepsilon_n = \frac{1}{2} \left[\frac{A+\alpha(\alpha-1)}{n-\alpha+1} - (n-\alpha+1) \right]$ and for $\alpha > 1/2$:

$$\left\{ \begin{array}{l} E_n = -\frac{\hbar^2}{8\mu b^2} \left[\frac{A+\alpha(\alpha-1)}{n+\alpha} - (n+\alpha) \right]^2; \\ n = 0, 1, 2, \dots, n_{\max} = \left[\sqrt{A + \alpha(\alpha-1)} - \alpha \right] \text{ and} \\ u_{n0}(r) = \tilde{\mathcal{N}}_n e^{-(\varepsilon'_n/b)r} (1 - e^{-r/b})^\alpha \\ {}_2F_1(-n, n + 2(\varepsilon'_n + \alpha); 2\varepsilon'_n + 1; e^{-r/b}), \end{array} \right. \quad (26)$$

where $\varepsilon'_n = \frac{1}{2} \left[\frac{A+\alpha(\alpha-1)}{n+\alpha} - (n+\alpha) \right]$. The normalization constants \mathcal{N}_n and $\tilde{\mathcal{N}}_n$ are calculated explicitly in the Appendix B. Notice that n_{\max} is the number of bound states for the whole bound spectrum near the continuous zone. n_{\max} is the largest integer which is less than or equal to the value of n that makes the right side of Eqs. (25) and (26) to vanish. The above results are identical to Eqs. (12) and (13) given by Ref. [34].

III. APPLICATIONS TO DIATOMIC MOLECULES

To show the accuracy of the new approximation scheme, we have calculated the ro-vibrational energy spectra for various n and l quantum numbers with two different values of the parameters α . The results obtained by means of Eq. (19) are compared with those obtained by a MATHEMATICA package programmed by Lucha and Schöberl [28] as listed in Table 1 for short-range (large b) and long-range (small b) potentials. This is an illustration to assess the validity and usefulness of our present approximations. The results of the energy spectrum for p -state show that the percentage accuracy decreases as either n or $1/b$ increases, for example, when $1/b = 0.025$, then the range of accuracies can be as follows: 0.00075%, 0.00087%, 0.0014%, 0.017% and 0.11% for $n = 0, 1, 2, 3$, and 4, respectively. However, when $1/b$ changes between 0.025 – 0.075, then the range of accuracies can be 0.00075% – 0.0022%, 0.00087% – 0.068%, 0.0014% – 1.57% for $n = 0, 1$ and 2, respectively. In addition, we present the ro-vibrational energy states for a few diatomic molecules HCl, CH, LiH, CO, NO, O₂, I₂, N₂, H₂ and Ar₂ in Tables 2-6. Lowest eigenvalues of $l = 0, 1, 2, 3$ are given at four values of $1/b$ in the range 0.025 – 0.1 covering both weaker and stronger interaction to demonstrate the generality of our results. The formalism is quite simple, computationally efficient, reliable and illustrated very accurate.

IV. SOME SPECIAL CASES

Let us study a few special cases. In the case where $\alpha = 0$ or $\alpha = 1$, the MR potential (1) reduces to the Hulthén potential [9,11]:

$$V^{(H)}(r) = -V_0 \frac{e^{-\delta r}}{1 - e^{-\delta r}}, \quad V_0 = Ze^2\delta, \quad \delta = b^{-1}, \quad (27)$$

where Ze^2 is the strength and δ 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. Furthermore, if taking $b = 1/\delta$ and identifying $(A\hbar^2/2\mu b^2)$ as $Ze^2\delta$, we are able to obtain the ro-vibrating energy states and the normalized wavefunctions deduced from Eqs. (19) and (24), respectively,

$$E_{nl} = -\frac{\hbar^2\delta^2}{2\mu} \left[\frac{(2\mu Ze^2/\hbar^2\delta) + l(l+1)(D_2 - D_1)}{2n+1 + \sqrt{1+4l(l+1)D_2}} - \frac{2n+1 + \sqrt{1+4l(l+1)D_2}}{4} \right]^2$$

$$+ \frac{\hbar^2 \delta^2 l(l+1) D_0}{2\mu}, \quad 0 \leq n, l < \infty, \quad (28)$$

and

$$u_{nl}(r) = \mathcal{N}_{nl} e^{-(\varepsilon_{nl}/b)r} (1 - e^{-r/b})^{\nu_l} {}_2F_1 \left(-n, n + 2(\varepsilon_{nl} + \nu_l); 2\varepsilon_{nl} + 1; e^{-r/b} \right),$$

$$\varepsilon_{nl} = \sqrt{-\frac{2\mu E_{n,l}}{\hbar^2 \delta^2} + l(l+1)D_0} > 0, \quad \nu_l = \frac{1}{2} \left(1 + \sqrt{1 + 4l(l+1)D_2} \right) \geq 1, \quad (29)$$

where \mathcal{N}_{nl} is given in the Appendix B. Also, for s -wave ($l = 0$) states, we get

$$E_n = -\frac{\mu (Ze^2)^2}{2\hbar^2} \left[\frac{1}{(n+1)} - \frac{\hbar^2 \delta}{2Ze^2 \mu} (n+1) \right]^2, \quad 0 \leq n < \infty. \quad (30)$$

and

$$u_n(r) = \mathcal{N}_n e^{-(\varepsilon_n/b)r} (1 - e^{-r/b}) {}_2F_1 \left(-n, n + 2(\varepsilon_n + 1); 2\varepsilon_n + 1; e^{-r/b} \right),$$

$$\varepsilon_n = \sqrt{-\frac{2\mu E_{n0}}{\hbar^2 \delta^2}} > 0, \quad (31)$$

where \mathcal{N}_n can be easily found from either relation (B7) or (B9) after setting $\alpha = 0$ or $\alpha = 1$ in the Appendix B, respectively. Here in this case $\varepsilon_n = \varepsilon'_n$ and the number of bound states n_{\max} is also same in both relations (B8) and (B10). In the usual approximation [19] where $D_0 = 0$ and $D_1 = D_2 = 1$, Eqs. (28) and (29) turn out to become

$$E_{nl} = -\frac{\mu (Ze^2)^2}{2\hbar^2} \left[\frac{1}{(n+l+1)} - \frac{\hbar^2 \delta}{2\mu Ze^2} (n+l+1) \right]^2, \quad 0 \leq n, l < \infty, \quad (32)$$

and

$$u_{nl}(r) = \mathcal{N}_{nl} e^{-(\varepsilon_{nl}/b)r} (1 - e^{-r/b})^{l+1} {}_2F_1 \left(-n, n + 2(\varepsilon_{nl} + l + 1); 2\varepsilon_{nl} + 1; e^{-r/b} \right),$$

$$\varepsilon_{nl} = \sqrt{-\frac{2\mu E_{nl}}{\hbar^2 \delta^2}} > 0, \quad (33)$$

where \mathcal{N}_{nl} can be found from relation (B6) by setting $\nu_l = l + 1$. Essentially, these results coincide with those obtained by the Feynman integral method [17] and the standard way [18,19]. In following Ref. [27] by taking $D_1 = D_2 = 1$ and $D_0 = 1/12$, Eqs. (28) and (29) turn out to become

$$E_{nl} = -\frac{\mu (Ze^2)^2}{2\hbar^2} \left[\frac{1}{(n+l+1)} - \frac{\hbar^2 \delta}{2\mu Ze^2} (n+l+1) \right]^2 + \frac{l(l+1)\hbar^2 \delta^2}{24\mu}, \quad 0 \leq n, l < \infty, \quad (34)$$

and

$$u_{nl}(r) = \mathcal{N}_{nl} e^{-(\varepsilon_{nl}/b)r} (1 - e^{-r/b})^{l+1} {}_2F_1 \left(-n, n + 2(\varepsilon_{nl} + l + 1); 2\varepsilon_{nl} + 1; e^{-r/b} \right),$$

$$\varepsilon_{nl} = \sqrt{-\frac{2\mu E_{nl}}{\hbar^2 \delta^2} + \frac{l(l+1)}{12}} > 0, \quad (35)$$

which coincide for the ground state with Gönül *et al.* [9] in Eq. (6). The Hulthén potential behaves like the Coulomb potential near the origin ($r \rightarrow 0$), but in the asymptotic region ($r \gg 1$) the Hulthén potential decreases exponentially, so its capacity for bound states is smaller than the Coulomb potential. However, for small values of the screening parameter or for $\delta r \ll 1$ (i.e., $r/b \ll 1$), the Hulthén potential becomes the Coulomb potential given by : $V_C(r) = -\frac{Ze^2}{r}$ with energy levels and wave functions:

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

$$\varepsilon_0 = \frac{Z^2 \hbar^2}{2\mu a_0^2}, \quad a_0 = \frac{\hbar^2}{\mu e^2} \quad (36)$$

where $\varepsilon_0 = 13.6 \text{ eV}$ and a_0 is Bohr radius for the Hydrogen atom [3]. The wave functions also take the form:

$$u_{nl}(r) = N_{nl} \exp \left[-\frac{\mu Z e^2}{\hbar^2} \frac{r}{(n+l+1)} \right] r^{l+1} P_n \left(\frac{2\mu Z e^2}{\hbar^2 \delta (n+l+1)}, 2l+1 \right) (r), \quad (37)$$

which are found identical to Refs. [11,13].

V. COCLUSIONS

We have applied an alternative improved approximation scheme of the centrifugal potential $l(l+1)r^{-2}$ to obtain the energy levels and corresponding wavefunctions for the MR potential in the framework of the NU method for arbitrary l -waves. We have calculated the bound state energy eigenvalues for the MR potential with $\alpha = 0.75, 1.5$ and $A = 2b$ and several $1/b$ screening parameter values. The wave functions are physical and bound state energies are in good agreement with the results obtained by other methods for short-range potential, small α and l . The precision of the resulting approximation of the wave functions (24) for the $V_{\text{eff}}(r)$ in Eq. (5b) is due to approximative character of the centrifugal term $1/r^2$ in Eq. (6) for $l \neq 0$ states since the wave functions are relevant to the bound state energy approximation in Eq. (19). The approximation (6) for the centrifugal potential allows to get analytic approximation (34) and (35) for the eigenvalues and the eigenfunctions for the MR

potential in the framework of the NU method for arbitrary l -waves. It is not possible to compute the residual (the error in the solution $u_{nl}^{(\text{approx})}(r)$ given by Eq. (24)) since the correct (exact) wave functions, $u_{nl}^{(\text{correct})}(r)$ of Eq. (5) are still not found. Hence, the notation residual can be used for $R = Hu_{nl}^{(\text{approx})}(r) - E_{nl}^{(\text{approx})}u_{nl}^{(\text{approx})}(r)$ and the error (or deviation) for the difference $u_{nl}^{(\text{exact})}(r) - u_{nl}^{(\text{approx})}(r)$ and $E_{nl}^{(\text{exact})} - E_{nl}^{(\text{approx})}$. Due to the slowness of the numerical calculation of the Hypergeometric functions ${}_2F_1(-n, n + 2(\varepsilon_{nl} + \nu_l); 2\varepsilon_{nl} + 1; e^{-r/b})$ and their derivatives in MATHEMATICA, the residual R is not evaluated. This residual is expected to be 6 order of magnitude smaller than typical values $E_{nl}^{(\text{approx})}u_{nl}^{(\text{approx})}(r)$. Accordingly, the error $u_{nl}^{(\text{exact})}(r) - u_{nl}^{(\text{approx})}(r)$ is expected to be also small. Furthermore, the error of approximation of the Hamiltonian (4) with potential (5) is already smaller, since the approximation used in (6) is only valid when $r \ll b$ (small screening parameter $\delta = 1/b$). In order to demonstrate this, NU results have been compared with the results of the numerical integration procedures using the MATHEMATICA program [28] and the results obtained from usual approximations scheme of the centrifugal potential [26]. For small $1/b$ values, NU results are in high agreement with the ones obtained in [28], but in the high screening region (large $1/b$ values) the agreement is poor. It is obvious from Table 1 that five (three) decimal digits are expected to be correct in the present (previous) approximation. The reason is simply that when r/b increases in the high-screening region, the agreement between the approximation expression and the centrifugal potential decreases. We have also studied two special cases for $l = 0$, $l \neq 0$ and Hulthén potential. As we have seen, NU method puts no constraint on the potential parameter values involved and is easy to implement. Our results are sufficiently accurate for the practical purposes. Therefore, we have applied the present solution in Eq. (19) to obtain the ro-vibrational energies ($-E_{nl}$) for the HCl, CH, LiH, CO, NO, O₂, I₂, N₂, H₂ and Ar₂ diatomic molecules.

Acknowledgments

The author wishes to thank the anonymous referees for their enlightening comments and suggestions. The support provided by the Scientific and Technological Research Council of Turkey (TÜBİTAK) is highly appreciated.

Appendix A: Normalization for the radial wave functions

The normalization constant, \mathcal{N}_{nl} can be determined in closed form. We start by using the relation between the hypergeometric function and the Jacobi polynomials (see formula (8.962.1) in [35]):

$${}_2F_1 \left(-n, n + \nu + \mu + 1; \nu + 1; \frac{1-x}{2} \right) = \frac{n!}{(\nu + 1)_n} P_n^{(\nu, \mu)}(x),$$

$$(\nu + 1)_n = \frac{\Gamma(n + \nu + 1)}{\Gamma(\nu + 1)}, \quad (\text{A1})$$

to rewrite the wave functions in (24) as

$$u_{nl}(r) = \mathcal{N}_{nl} \frac{n! \Gamma(2\varepsilon_{nl} + 1)}{\Gamma(n + 2\varepsilon_{nl} + 1)} e^{-\varepsilon_{nl} r/b} (1 - e^{-r/b})^{\nu_l} P_n^{(2\varepsilon_{nl}, 2\nu_l - 1)}(1 - 2e^{-r/b}). \quad (\text{A2})$$

From the normalization condition $\int_0^\infty [u_{nl}(r)]^2 dr = 1$ and under the coordinate change $x = 1 - 2e^{-r/b}$, the normalization constant in (B2) is given by

$$\mathcal{N}_{nl}^{-2} = b \left[\frac{n! \Gamma(2\varepsilon_{nl} + 1)}{\Gamma(n + 2\varepsilon_{nl} + 1)} \right]^2 \int_{-1}^1 \left(\frac{1-x}{2} \right)^{2\varepsilon_{nl}} \left(\frac{1+x}{2} \right)^{2\nu_l - 1} \left(\frac{1+x}{2} \right) [P_n^{(2\varepsilon_{nl}, 2\nu_l - 1)}(x)]^2 dx. \quad (\text{A3})$$

The calculation of this integral can be done by writting

$$\frac{1+x}{2} = 1 - \left(\frac{1-x}{2} \right),$$

and by making use of the following two integrals (see formula (7.391.5) in [35]):

$$\int_{-1}^1 (1-x)^{\nu-1} (1+x)^\mu [P_n^{(\nu, \mu)}(x)]^2 dx = 2^{\nu+\mu} \frac{\Gamma(n + \nu + 1) \Gamma(n + \mu + 1)}{n! \nu \Gamma(n + \nu + \mu + 1)}, \quad (\text{A4})$$

which is valid for $\mathcal{R}e(\nu) > 0$ and $\mathcal{R}e(\mu) > -1$ and (see formula (7.391.1) in [35]):

$$\int_{-1}^1 (1-x)^\nu (1+x)^\mu [P_n^{(\nu, \mu)}(x)]^2 dx = 2^{\nu+\mu+1} \frac{\Gamma(n + \nu + 1) \Gamma(n + \mu + 1)}{n! \Gamma(n + \nu + \mu + 1) (2n + \nu + \mu + 1)}, \quad (\text{A5})$$

which is valid for $\mathcal{R}e(\nu) > -1$, $\mathcal{R}e(\mu) > -1$. This leads to

$$\mathcal{N}_{nl} = \frac{1}{\Gamma(2\varepsilon_{nl} + 1)} \left[\frac{\varepsilon_{nl}(n + \varepsilon_{nl} + \nu_l)}{2b(n + \nu_l)} \frac{\Gamma(n + 2\varepsilon_{nl} + 1) \Gamma(n + 2\varepsilon_{nl} + 2\nu_l)}{n! \Gamma(n + 2\nu_l)} \right]^{1/2}, \quad (\text{A6})$$

where $0 \leq n, l < \infty$. In the s -wave ($l = 0$) case, the above result is written explicitly, for $\alpha < 1/2$:

$$\mathcal{N}_n = \frac{1}{\Gamma(2\varepsilon_n + 1)} \left[\frac{\varepsilon_n(n + \varepsilon_n - \alpha + 1)}{2b(n - \alpha + 1)} \frac{\Gamma(n + 2\varepsilon_n + 1) \Gamma(n + 2\varepsilon_n - 2\alpha + 2)}{n! \Gamma(n - 2\alpha + 2)} \right]^{1/2}, \quad (\text{A7})$$

where

$$\varepsilon_n = \frac{A + \alpha(\alpha - 1)}{2(n - \alpha + 1)} - \frac{n - \alpha + 1}{2}, \quad 0 \leq n < n_{\max} = \left[\sqrt{A + \alpha(\alpha - 1)} + \alpha - 1 \right] \quad (\text{A8})$$

in which $\alpha = 0$ is included in $(-\infty, 1/2)$ and for $\alpha > 1/2$:

$$\tilde{\mathcal{N}}_n = \frac{1}{\Gamma(2\varepsilon_n + 1)} \left[\frac{\varepsilon'_n(n + \varepsilon'_n + \alpha)}{2b(n + \alpha)} \frac{\Gamma(n + 2\varepsilon'_n + 1)\Gamma(n + 2\varepsilon'_n + 2\alpha)}{n!\Gamma(n + 2\alpha)} \right]^{1/2}, \quad (\text{A9})$$

where

$$\varepsilon'_n = \frac{A + \alpha(\alpha - 1)}{2(n + \alpha)} - \frac{n + \alpha}{2}, \quad 0 \leq n < n_{\max} = \left[\sqrt{A + \alpha(\alpha - 1)} - \alpha \right]. \quad (\text{A10})$$

in which $\alpha = 1$ is included in $(1/2, \infty)$.

-
- [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] S. Ikhdaïr and R. Sever, J. Mol. Struct.-Theochem 806 (2007) 155.
- [5] S.M. Ikhdaïr and R. Sever, J. Mol. Struct.-Theochem 855 (2008) 13.
- [6] C.L. Pekeris, Phys. Rev. 45 (1934) 98; C. Berkdemir, Nucl. Phys. A 770 (2006) 32.
- [7] W.-C. Qiang and S.-H. Dong, Phys. Lett. A 363 (2007) 169.
- [8] C. Berkdemir and J. Han, Chem. Phys. Lett. 409 (2005) 203; C. Berkdemir, A. Berkdemir and J. Han, Chem. Phys. Lett. 417 (2006) 326.
- [9] R.L. Greene and C. Aldrich, Phys. Rev. A 14 (1976) 2363; B. Gönül and İ. Zorba, Phys. Lett. A 269 (2000) 83.
- [10] P.M. Morse, Phys. Rev. 34 (1929) 57; S.M. Ikhdaïr, Chem. Phys. 361 (1-2) (2009) 9.
- [11] L. Hulthén, Ark. Mat. Astron. Fys. A 28 (1942) 5; S.M. Ikhdaïr and R. Sever, J. Math. Chem. 42 (3) (2007) 461.
- [12] Ö. Yeşiltaş, Phys. Scr. 75 (2007) 41.
- [13] S.M. Ikhdaïr and R. Sever, Int. J. Mod. Phys. A 25 (2010) 3941; S.M. Ikhdaïr and R. Sever, Cent. Eur. J. Phys. 8 (2010) 652; S.M. Ikhdaïr and R. Sever, Int. J. Theor. Phys. 46 (2007) 1643.
- [14] S.M. Ikhdaïr, Chin. J. Phys. 46 (2008) 291; S.M. Ikhdaïr and R. Sever, Int. J. Mod. Phys. C 18 (2007) 1571; S.M. Ikhdaïr and R. Sever, Int. J. Mod. Phys. C 19 (2008) 221; S.M. Ikhdaïr and R. Sever, Cent. Eur. J. Phys. 5 (2007) 516; S.M. Ikhdaïr and R. Sever, Cent. Eur. J. Phys. 6 (2008) 141, 685; 697; S.M. Ikhdaïr and R. Sever, Int. J. Mod. Phys. C 19 (2008) 1425; S.M. Ikhdaïr and R. Sever, J. Math. Chem. 45 (2009) 1137.
- [15] S.M. Ikhdaïr, J. Math. Phys. 51 (2010) 023525; N. Rosen and P.M. Morse, Phys. Rev. 42 (1932) 210.
- [16] M.F. Manning, Phys. Rev. 44 (1933) 951; M.F. Manning and N. Rosen, Phys. Rev. 44 (1933) 953.
- [17] A. Diaf, A. Chouchaoui and R.L. Lombard, Ann. Phys. (Paris) 317 (2005) 354.

- [18] S.-H. Dong and J. Garcia-Ravelo, *Phys. Scr.* 75 (2007) 307.
- [19] W.-C. Qiang and S. H. Dong, *Phys. Lett. A* 368 (2007) 13.
- [20] C.-S. Jia *et al.*, *J. Phys. A: Math. Gen.* 37 (2004) 11275; C.-S. Jia *et al.*, *Phys. Lett. A* 311 (2003) 115.
- [21] H. Eğrifles, D. Demirhan and F. Büyükkılıç, *Phys. Lett. A* 275 (2000) 229.
- [22] W.-C. Qiang, *Chin. Phys.* 12 (2003) 1054; *ibid.* 13 (2004) 575; L.-Z. Yi, Y.-F. Diao, J.-Y. Liu and C.-S. Jia, *Phys. Lett. A* 333 (2004) 212; G.-F. Wei and S.-H. Dong, *Phys. Lett. A* 373 (2008) 49.
- [23] R.J. Le Roy and R.B. Bernstein, *J. Chem. Phys.* 52 (1970) 3869.
- [24] J. Cai, P. Cai and A. Inomata, *Phys. Rev. A* 34 (1986) 4621.
- [25] G.F. Wei, C.Y. Long and S.H. Dong, *Phys. Lett. A* 372 (2008) 2592.
- [26] S.M. Ikhdair and R. Sever, *Ann. Phys. (Berlin)* 17 (2008) 897; S.M. Ikhdair and R. Sever, *Phys. Scr.* 79 (2009) 035002.
- [27] S.M. Ikhdair, *Eur. Phys. J. A* 39 (2009) 307.
- [28] W. Lucha and F.F. Schöberl, *Int. J. Mod. Phys. C* 10 (1999) 607.
- [29] S.M. Ikhdair and R. Sever, to appear in the *Int. J. Mod. Phys. B* (2011) [arXiv:0909.0623]; S.M. Ikhdair and R. Sever, *Ann. Phys. (Berlin)* 18 (2009) 747.
- [30] A.F. Nikiforov and V.B. Uvarov, *Special Functions of Mathematical Physics* (Birkhauser, Basel, 1988).
- [31] S.M. Ikhdair and R. Sever, *Appl. Math. Comp.* 216 (2010) 911.
- [32] G.-F. Wei and S.-H. Dong, *Phys. Lett. A* 373 (2008) 49.
- [33] S.M. Ikhdair, *Chem. Phys.* 361 (2009) 9.
- [34] F. Benamira, L. Guechi and A. Zouache, *Phys. Scr.* 80 (2009) 017001.
- [35] I.S. Gradshteyn and I.M. Ryzhik, *Tables and integrals, series and products* (New York, Academic, 1969).

TABLE I: Bound state energy spectrum ($-E_{nl}$) (in atomic units) for the Manning-Rosen potential as a function of $1/b$ for $2p, 3p, 3d, 4p, 4d, 4f, 5p, 5d, 5f, 5g, 6p, 6d, 6f$ and $6g$ states with $\alpha = 0.75$, $\alpha = 1.5$ and $A = 2b$.

states	$1/b$	$\alpha = 0.75$			$\alpha = 1.5$		
		present	previous [26]	Lucha et al [28]	present	previous [26]	Lucha et al [28]
$2p$	0.025	0.1205279	0.1205793	0.1205271	0.0899715	0.0900229	0.0899708
	0.050	0.1082170	0.1084228	0.1082151	0.0800414	0.0802472	0.0800400
	0.075	0.0964490	0.0969120	0.0964469	0.0705703	0.0710332	0.0705701
	0.100	0.0852240	0.0860740		0.0615579	0.0577157	
$3p$	0.025	0.0458783	0.0459297	0.0458779	0.0369137	0.0369651	0.0369134
	0.050	0.0350614	0.0352672	0.0350633	0.0272662	0.0274719	0.0272696
	0.075	0.0255480	0.0260110	0.0255654	0.0189220	0.0193850	0.0189474
	0.100	0.0173379	0.0181609		0.0118813	0.0127043	
$3d$	0.025	0.0447756	0.0449299	0.0447743	0.0394801	0.0396345	0.0394789
	0.050	0.0336909	0.0343082	0.0336930	0.0294456	0.0300629	0.0294496
	0.075	0.0237279	0.0251168	0.0237621	0.0204232	0.0218121	0.0204663
$4p$	0.025	0.0208094	0.0208608	0.0208097	0.0171735	0.0172249	0.0171740
	0.050	0.0117234	0.0119292	0.0117365	0.0088961	0.0091019	0.0089134
	0.075	0.0050143	0.0054773	0.0050945	0.0030849	0.0035478	0.0031884
$4d$	0.025	0.0203012	0.0204555	0.0203017	0.0182106	0.0183649	0.0182115
	0.050	0.0109569	0.0115742	0.0109904	0.0094775	0.0100947	0.0095167
	0.075	0.0038158	0.0052047	0.0040331	0.0028919	0.0042808	0.0031399
$4f$	0.025	0.0199801	0.0202887	0.0199797	0.0186136	0.0189223	0.0186137
	0.050	0.0101938	0.0114284	0.0102393	0.0093507	0.0105852	0.0094015
	0.075	0.0023157	0.0050935	0.0026443	0.0018749	0.0046527	0.0022307
$5p$	0.025	0.0098062	0.0098576	0.0098079	0.0080793	0.0081308	0.0080816
$5d$	0.025	0.0095094	0.0096637	0.0095141	0.0085359	0.0086902	0.0085415
$5f$	0.025	0.0092751	0.0095837	0.0092825	0.0086536	0.0089622	0.0086619
$5g$	0.025	0.0090254	0.0095398	0.0090330	0.0086066	0.0091210	0.0086150
$6p$	0.025	0.0043537	0.0044051	0.0043583	0.0034820	0.0035334	0.0034876
$6d$	0.025	0.0041518	0.0043061	0.0041650	0.0036666	0.0038209	0.0036813
$6f$	0.025	0.0039566	0.0042652	0.0039803	0.0036520	0.0039606	0.0036774
$6g$	0.025	0.0037284	0.0042428	0.0037611	0.0035278	0.0040422	0.0035623

TABLE II: The ro-vibrational energy spectra ($-E_{nl}$) (in eV) for HCl and CH for $2p, 3p, 3d, 4p, 4d, 4f, 5p, 5d, 5f, 5g, 6p, 6d, 6f$ and $6g$ states with $\hbar c = 1973.29 eV \text{ \AA}^\circ$, $\mu_{\text{HCl}} = 0.9801045 \text{ amu}$, $\mu_{\text{CH}} = 0.929931 \text{ amu}$ 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	4.80933	5.14059	3.83734	5.06882	5.41795	4.04438
	0.050	4.30960	4.61553	3.41382	4.54212	4.86455	3.59801
	0.075	3.83214	4.11362	3.00987	4.03890	4.33556	3.17226
	0.100	3.37695	3.63486	2.42549	3.55915	3.83097	2.76714
$3p$	0.025	1.86414	1.95674	1.57439	1.96472	2.06231	1.65934
	0.050	1.41439	1.49539	1.16292	1.49071	1.57608	1.22566
	0.075	1.02023	1.08964	0.80704	1.07528	1.14843	0.85058
	0.100	0.68166	0.73947	0.50674	0.71844	0.77937	0.53409
$3d$	0.025	1.85975	1.90971	1.68385	1.96010	2.01275	1.77470
	0.050	1.39684	1.43694	1.25588	1.47221	1.51447	1.32363
	0.075	0.98074	1.01201	0.87106	1.03366	1.06661	0.91806
	0.100	0.61146	0.63492	0.52941	0.64445	0.66917	0.55798
$4p$	0.025	0.85082	0.88753	0.73246	0.89672	0.93542	0.77198
	0.050	0.47104	0.50001	0.37942	0.496459	0.526989	0.399896
	0.075	0.19351	0.21387	0.13157	0.203948	0.225404	0.138671
$4d$	0.025	0.84643	0.86586	0.77669	0.892099	0.912577	0.818599
	0.050	0.45349	0.46732	0.40422	0.477960	0.492531	0.426029
	0.075	0.15402	0.16275	0.12334	0.162325	0.171527	0.129997
$4f$	0.025	0.83985	0.85216	0.79388	0.885162	0.898138	0.836716
	0.050	0.42716	0.43477	0.39881	0.450211	0.458228	0.420329
	0.075	0.094777	0.098765	0.079967	0.099891	0.104094	0.084281
$5p$	0.025	0.40099	0.41824	0.34459	0.422623	0.440805	0.363181
$5d$	0.025	0.39660	0.40558	0.36406	0.417998	0.427463	0.383705
$5f$	0.025	0.390018	0.395586	0.36908	0.411061	0.416929	0.388993
$5g$	0.025	0.381242	0.38494	0.367077	0.401811	0.405709	0.386882
$6p$	0.025	0.176998	0.18569	0.14851	0.186548	0.195706	0.156521
$6d$	0.025	0.172610	0.17708	0.15638	0.181923	0.186631	0.164820
$6f$	0.025	0.166028	0.168752	0.155759	0.174986	0.177856	0.164163
$6g$	0.025	0.157252	0.15902	0.150462	0.165736	0.167600	0.158580

TABLE III: The ro-vibrational energy spectra ($-E_{nl}$) (in eV) for LiH and CO for $2p, 3p, 3d, 4p, 4d, 4f, 5p, 5d, 5f, 5g, 6p, 6d, 6f$ and $6g$ states with $\mu_{\text{LiH}} = 0.8801221 \text{ amu}$, $\mu_{\text{CO}} = 6.8606719 \text{ amu}$ 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	5.35568	5.72457	4.27326	0.687053	0.734377	0.548196	
	0.050	4.79918	5.13985	3.80163	0.615663	0.659367	0.487693	
	0.075	4.26747	4.58092	3.35179	0.547453	0.587664	0.429985	
	0.100	3.76057	4.04778	2.92374	0.482425	0.519270	0.375073	
$3p$	0.025	2.07591	2.17902	1.75324	0.266308	0.279536	0.224915	
	0.050	1.57507	1.66527	1.29503	0.202058	0.213629	0.166133	
	0.075	1.13613	1.21342	0.89872	0.145749	0.155664	0.115292	
	0.100	0.759101	0.823478	0.564311	0.097381	0.105640	0.072393	
$3d$	0.025	2.07102	2.12665	1.87514	0.265681	0.272818	0.240553	
	0.050	1.55552	1.60018	1.39854	0.199550	0.205279	0.179412	
	0.075	1.09215	1.12698	0.970015	0.140107	0.144574	0.124439	
	0.100	0.680918	0.707045	0.589556	0.087352	0.090703	0.075631	
$4p$	0.025	0.947473	0.988358	0.815668	0.121547	0.126792	0.104638	
	0.050	0.524555	0.556813	0.422528	0.067293	0.071431	0.054204	
	0.075	0.215490	0.238160	0.146518	0.027644	0.030552	0.018796	
$4d$	0.025	0.942586	0.964223	0.864926	0.120920	0.123695	0.110957	
	0.050	0.505009	0.520405	0.450139	0.064785	0.066760	0.057746	
	0.075	0.171512	0.181234	0.137354	0.022002	0.023250	0.017620	
$4f$	0.025	0.935256	0.948967	0.884069	0.119979	0.121738	0.113413	
	0.050	0.475690	0.484161	0.444117	0.061024	0.062111	0.056974	
	0.075	0.105544	0.109984	0.089051	0.013540	0.014109	0.011424	
$5p$	0.025	0.446540	0.465751	0.383735	0.057284	0.059749	0.049227	
$5d$	0.025	0.441654	0.451655	0.405420	0.056658	0.057941	0.052009	
$5f$	0.025	0.434324	0.440525	0.411008	0.055717	0.056513	0.052726	
$5g$	0.025	0.424551	0.428669	0.408777	0.054464	0.054992	0.052440	
$6p$	0.025	0.197105	0.206782	0.165379	0.025286	0.026527	0.021216	
$6d$	0.025	0.192219	0.197193	0.174148	0.024659	0.025297	0.022341	
$6f$	0.025	0.184889	0.187922	0.173454	0.023718	0.024108	0.022252	
$6g$	0.025	0.175116	0.177085	0.167554	0.022465	0.022717	0.021495	

TABLE IV: The ro-vibrational energy spectra ($-E_{nl}$) (in eV) for NO and O₂ for $2p, 3p, 3d, 4p, 4d, 4f, 5p, 5d, 5f, 5g, 6p, 6d, 6f$ and $6g$ states with $\mu_{\text{NO}} = 7.468441 \text{ amu}$, $\mu_{\text{O}_2} = 7.997457504 \text{ amu}$ and $A = 2b$.

states	$1/b^a$	NO/ $\alpha = 0, 1$	$\alpha = 0.75$	$\alpha = 1.5$	O ₂ / $\alpha = 0, 1$	$\alpha = 0.75$	$\alpha = 1.5$
$2p$	0.025	0.631142	0.674615	0.503585	0.589393	0.629990	0.470274
	0.050	0.565561	0.605709	0.448005	0.528150	0.565642	0.418370
	0.075	0.502903	0.539841	0.394993	0.469637	0.504132	0.368865
	0.100	0.443166	0.477013	0.344550	0.413852	0.445459	0.321759
$3p$	0.025	0.244637	0.256788	0.206612	0.228454	0.239802	0.192945
	0.050	0.185615	0.196245	0.152613	0.173337	0.183263	0.142518
	0.075	0.133888	0.142996	0.105910	0.125032	0.133537	0.098904
	0.100	0.089457	0.097043	0.066502	0.083539	0.090624	0.062103
$3d$	0.025	0.244061	0.250617	0.220977	0.227917	0.234039	0.206360
	0.050	0.183311	0.188574	0.164812	0.171186	0.176100	0.153910
	0.075	0.128706	0.132809	0.114312	0.120192	0.124024	0.106750
	0.100	0.080243	0.083322	0.069477	0.074935	0.077810	0.064881
$4p$	0.025	0.111655	0.116474	0.096123	0.104270	0.108769	0.089764
	0.050	0.061816	0.065618	0.049793	0.057727	0.061277	0.046499
	0.075	0.025395	0.028066	0.017267	0.023715	0.026210	0.016124
$4d$	0.025	0.111080	0.113629	0.101928	0.103732	0.106113	0.095185
	0.050	0.059513	0.061327	0.053047	0.055576	0.057271	0.049538
	0.075	0.020212	0.021358	0.016187	0.018875	0.019945	0.015116
$4f$	0.025	0.110216	0.111831	0.104184	0.102925	0.104434	0.097292
	0.050	0.056058	0.057056	0.052337	0.052350	0.053282	0.048875
	0.075	0.012438	0.012961	0.010494	0.011615	0.012104	0.009800
$5p$	0.025	0.052623	0.054887	0.045221	0.049142	0.051256	0.042230
$5d$	0.025	0.052047	0.053225	0.047777	0.048604	0.049705	0.044617
$5f$	0.025	0.051183	0.051914	0.048435	0.047797	0.048480	0.045231
$5g$	0.025	0.050031	0.050517	0.048173	0.046722	0.047175	0.044986
$6p$	0.025	0.023228	0.024368	0.019489	0.021691	0.022756	0.018200
$6d$	0.025	0.022652	0.023238	0.020523	0.021154	0.021701	0.019165
$6f$	0.025	0.021788	0.022146	0.020441	0.020347	0.020681	0.019089
$6g$	0.025	0.020637	0.020869	0.019746	0.019272	0.019488	0.018439

TABLE V: The ro-vibrational energy spectra ($-E_{nl}$) (in eV) for I_2 and N_2 for $2p, 3p, 3d, 4p, 4d, 4f, 5p, 5d, 5f, 5g, 6p, 6d, 6f$ and $6g$ states with $\mu_{I_2} = 63.45223502 \text{ amu}$, $\mu_{N_2} = 7.00335 \text{ amu}$ and $A = 2b$.

states	$1/b^a$	$I_2/ \alpha = 0, 1$	$\alpha = 0.75$	$\alpha = 1.5$	$N_2/ \alpha = 0, 1$	$\alpha = 0.75$	$\alpha = 1.5$
$2p$	0.025	0.0742866	0.0794033	0.0592729	0.673056	0.719416	0.537028
	0.050	0.0665676	0.0712930	0.0527310	0.603120	0.645934	0.477757
	0.075	0.0591925	0.0635403	0.0464914	0.536300	0.575692	0.421225
	0.100	0.0521615	0.0561452	0.0405541	0.472597	0.508691	0.367431
$3p$	0.025	0.0287942	0.0302244	0.0243186	0.260883	0.273841	0.220333
	0.050	0.0218472	0.0230983	0.0179628	0.197941	0.209277	0.162748
	0.075	0.0157589	0.0168309	0.0124658	0.142780	0.152493	0.112943
	0.100	0.0105292	0.0114221	0.0078274	0.095397	0.103488	0.070918
$3d$	0.025	0.0287264	0.0294980	0.0260094	0.260269	0.267260	0.235652
	0.050	0.0215761	0.0221955	0.0193987	0.195485	0.201097	0.175757
	0.075	0.0151489	0.0156319	0.0134547	0.137253	0.141629	0.121903
	0.100	0.0094448	0.0098072	0.0081775	0.085572	0.088855	0.074090
$4p$	0.025	0.0131420	0.0137091	0.0113138	0.119070	0.124209	0.102506
	0.050	0.0072759	0.0072330	0.0058607	0.065922	0.069976	0.053100
	0.075	0.0029890	0.0033034	0.0020323	0.027081	0.029930	0.018413
$4d$	0.025	0.0130743	0.0133744	0.0119971	0.118456	0.121175	0.108697
	0.050	0.0070048	0.0072183	0.0062437	0.063465	0.065400	0.056570
	0.075	0.0023790	0.0025138	0.0019052	0.021554	0.022776	0.017261
$4f$	0.025	0.0129726	0.0131628	0.0122626	0.117535	0.119258	0.111102
	0.050	0.0065981	0.0067156	0.0061602	0.059781	0.060845	0.055813
	0.075	0.0014640	0.0015256	0.0012352	0.013264	0.013822	0.011191
$5p$	0.025	0.0061938	0.0064603	0.0053226	0.056117	0.058532	0.048225
$5d$	0.025	0.0061260	0.0062647	0.0056234	0.055503	0.056760	0.050950
$5f$	0.025	0.0060243	0.0061104	0.0057009	0.054582	0.055361	0.051652
$5g$	0.025	0.0058888	0.0059459	0.0056700	0.053354	0.053872	0.051372
$6p$	0.025	0.0027340	0.0028682	0.0022939	0.024771	0.025987	0.020783
$6d$	0.025	0.0026662	0.0027352	0.0024155	0.024156	0.024782	0.021885
$6f$	0.025	0.0025645	0.0026066	0.0024059	0.023235	0.023616	0.021798
$6g$	0.025	0.0024290	0.0024563	0.0023241	0.022007	0.022255	0.021057

TABLE VI: The ro-vibrational energy spectra ($-E_{nl}$) (in eV) for H_2 and Ar_2 for $2p, 3p, 3d, 4p, 4d, 4f, 5p, 5d, 5f, 5g, 6p, 6d, 6f$ and $6g$ states with $\mu_{H_2} = 0.50407 \text{ amu}$, $\mu_{Ar_2} = 19.9812 \text{ amu}$ and $A = 2b$.

states	$1/b^a$	$H_2/$	$\alpha = 0, 1$	$\alpha = 0.75$	$\alpha = 1.5$	$Ar_2/$	$\alpha = 0, 1$	$\alpha = 0.75$	$\alpha = 1.5$
$2p$	0.025	9.35118	9.99528	7.46126	0.235904	0.252153	0.188227		
	0.050	8.37951	8.97435	6.63777	0.211392	0.226398	0.167452		
	0.075	7.45114	7.99844	5.85233	0.187972	0.201778	0.147638		
	0.100	6.56608	7.06755	5.10495	0.165644	0.178295	0.128784		
$3p$	0.025	3.62460	3.80464	3.06122	0.091439	0.095981	0.077226		
	0.050	2.75012	2.90761	2.26116	0.069378	0.073351	0.057043		
	0.075	1.98372	2.11867	1.56919	0.050044	0.053448	0.039586		
	0.100	1.32541	1.43782	0.98531	0.033437	0.036272	0.024857		
$3d$	0.025	3.61607	3.71320	3.27405	0.0912234	0.0936738	0.0825953		
	0.050	2.71599	2.79396	2.44190	0.0685169	0.0704839	0.0616024		
	0.075	1.90694	1.96773	1.69368	0.0481067	0.0496405	0.0427268		
	0.100	1.18890	1.23452	1.02938	0.0299927	0.0311436	0.0259685		
$4p$	0.025	1.65432	1.72570	1.42418	0.041734	0.043535	0.035928		
	0.050	0.91589	0.97221	0.73775	0.023105	0.024526	0.018611		
	0.075	0.37625	0.41584	0.25583	0.0094918	0.0104904	0.0064538		
$4d$	0.025	1.64578	1.68356	1.51019	0.0415186	0.0424716	0.0380978		
	0.050	0.88176	0.90864	0.78596	0.0222444	0.0229225	0.0198275		
	0.075	0.29946	0.31644	0.23982	0.0075547	0.0079829	0.0060501		
$4f$	0.025	1.63299	1.65693	1.54361	0.0411957	0.0417996	0.0389410		
	0.050	0.83057	0.84536	0.77544	0.0209530	0.0213261	0.0195623		
	0.075	0.18428	0.19204	0.15549	0.0046490	0.0048445	0.0039225		
$5p$	0.025	0.77967	0.81322	0.67001	0.0196690	0.0205152	0.0169026		
$5d$	0.025	0.77114	0.78860	0.70788	0.0194538	0.0198943	0.0178578		
$5f$	0.025	0.75834	0.76917	0.71763	0.0191309	0.0194040	0.0181039		
$5g$	0.025	0.74128	0.74847	0.71374	0.0187004	0.0188818	0.0180056		
$6p$	0.025	0.34415	0.36105	0.28876	0.0086820	0.0091082	0.0072845		
$6d$	0.025	0.33562	0.34430	0.30407	0.0084667	0.0086859	0.0076708		
$6f$	0.025	0.32282	0.32812	0.30286	0.0081439	0.0827750	0.0076402		
$6g$	0.025	0.30576	0.30920	0.29256	0.0077134	0.0078001	0.0073804		