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

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Abstract
The approximate analytical bound-state solution of the Schrödinger equation for the Manning–Rosen (MR) potential is found 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 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 $\alpha$. 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 ($l = 0$) MR potential and the Hulthén potential are also studied.

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1. 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 for the Coulomb potential, the harmonic oscillator potential, the pseudoharmonic potentials, etc [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 approximation 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 potential [12], the Woods–Saxon potential [13], Kratzer-type and pseudoharmonic potentials [14], Rosen–Morse-type potentials [15], the Manning–Rosen (MR) potential [16–19] and other multiparameter exponential-type potentials [20, 21].

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

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

where $A$ and $\alpha$ are two constants and the parameter $b$ characterizes the range of the potential [22]. The above potential may be also put in the following simple form:

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

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...
by using the NU method. In section 4, is devoted to two special cases, namely s-wave \((l = 0)\) and the Hulthén potential. Finally, we make a few concluding remarks in section 5.

2. Bound-state solutions

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

\[
\left( \frac{\mu}{2m} + V(r) \right) \psi_{nlm}(r) = E_{nl} \psi_{nlm}(r),
\]

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

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

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

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

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

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

\[
\lim_{b \to \infty} \left[ \frac{1}{b^2} \left( D_0 + D_1 \frac{1}{(e^\beta r - 1)^2} + D_2 \frac{1}{(e^\beta r - 1)^2} \right) \right] = \frac{1}{r^2}, \tag{6b}
\]

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]

\[
D_0 \simeq \frac{1}{12}, \quad D_1 = D_2 = 1. \tag{7}
\]

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

\[
D_0 = \frac{12 \epsilon_1^2 - 4 \epsilon_1 (2A + 3 \epsilon_1) \log(\epsilon_2) + \epsilon_3^2 \log(\epsilon_2)^2}{\epsilon_3^2 \log(\epsilon_3)^4}, \tag{8a}
\]

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

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

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

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

\[
e_{nl} = \sqrt{\frac{2\mu b^2 E_{nl}}{\hbar^2}} + \Delta E_l > 0, \quad E_{nl} < \frac{\hbar^2}{2\mu b^2} \Delta E_l,
\]

\[
\Delta E_l = l(l + 1) D_0,
\]

\[
\beta_1 = A - l(l + 1) D_1,
\]

\[
\beta_2 = \alpha (\alpha - 1) + l(l + 1) D_2,
\]

to obtain the following compact hypergeometric equation:

\[
\frac{d^2u_{nl}(z)}{dz^2} + \frac{(1 - z) du_{nl}(z)}{dz} + \frac{1}{z(1 - z)} u_{nl}(z) + \left(-\epsilon_{nl}^2 + (2\epsilon_{nl}^2 + \beta_1) z - (\epsilon_{nl}^2 + \beta_1 + \beta_2) z^2\right) u_{nl}(z) = 0.
\]

Equation (10) with equation (1) of [33]; then we obtain the following definitions:

\[
\tilde{\epsilon}(z) = 1 - z, \quad \sigma(z) = z - z^2,
\]

\[
\tilde{\epsilon}(z) = -\epsilon_{nl}^2 + (2\epsilon_{nl}^2 + \beta_1) z - (\epsilon_{nl}^2 + \beta_1 + \beta_2) z^2.
\]

After applying relations (A.1)–(A.4) of [33], the following useful functions usually defined by the NU method [30] are achieved:

\[
k = \beta_1 - a\epsilon_{nl}, \quad a = \sqrt{(1 - 2\alpha)^2 + 4l(l + 1) D_2},
\]

\[
\pi(z) = -\frac{z}{2} - \frac{1}{2} [(a + 2\epsilon_{nl}) z - a]
\]

and

\[
\tau(z) = 1 + 2\epsilon_{nl} - (2 + 2\epsilon_{nl} + a) z, \quad \tau'(z) = -(2 + 2\epsilon_{nl} + a).
\]

We can also write the values of \( \lambda = k^2 \) and \( \lambda_n = -n \pi'(z) - \frac{n(n-1)}{2} \alpha^2(z), \) \( n = 0, 1, 2, \ldots \), to obtain

\[
\lambda = \beta_1 - (1 + a)(\frac{1}{2} + \epsilon_{nl}),
\]

\[
\lambda_n = n(1 + n + a + 2\epsilon_{nl}), \quad n = 0, 1, 2, \ldots.
\]

respectively. Furthermore, using the relation, \( \lambda = \lambda_n \), or alternatively the energy equation (A.5) of [33] allows one to obtain

\[
\epsilon_{nl} = \frac{A + \alpha(\alpha - 1) + l(l + 1) (D_2 - D_1)}{2n + 1 + a} - \frac{2n + 1 + a}{4}.
\]
Plugging the parameters given in equation (9) into (18), we finally obtain the following discrete bound-state energy eigenvalues:

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

(19)

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

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

(20)

Let us now turn to the calculation of the radial part of the normalized wave functions. After applying relations (A.6)–(A.10) of [33], we obtain

$$\phi(z) = z^{\epsilon_a}(1 - z)^{(1 + \alpha)/2},$$  

(21)

$$\rho(z) = z^{\epsilon_{\alpha}}(1 - z)^{\alpha},$$  

(22)

$$y_{nl}(z) = C_{nl}z^{-(\epsilon_a + 1)} \left( 1 - z \right)^{\alpha} \frac{d^n}{dz^n} \left[ z^{\alpha} \left( 1 - z \right)^{\alpha} \right].$$  

(23)

The functions $y_{nl}(z)$, up to a numerical factor, are in the form of Jacobi polynomials, i.e. $y_{nl}(z) \approx P_n^{(2\epsilon_a, \alpha)}(1 - z)$ (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 equations (5) are given by

$$u_{nl}(r) = u_{nl}^{(approx)}(r) = N_{nl}e^{-\epsilon_{\alpha}r/b}(1 - e^{-r/b})^{\nu};$$

$$\times 2 \frac{F_1(-n, n + 2, \epsilon_{nl} + \nu); 2\epsilon_{nl} + 1; e^{-r/b}}{\epsilon_{nl} > 0, \; \nu = (1 + \alpha) / 2 \geq 1},$$  

(24)

where $a$ and $\varepsilon_{nl}$ are given in equations (13) and (18), respectively, and $N_{nl}$ is a normalization constant determined in the appendix.

When $l = 0$, we deal with the $s$-wave case; the possible energies for the bound states and the corresponding wave
functions are written explicitly as follows:

for $\alpha < 1/2$

$$E_n = \frac{\hbar^2}{8\mu b^2} \left[ \frac{A + \alpha(n - 1)}{n - \alpha + 1} - (n - \alpha + 1) \right]^2,$$

$$n = 0, 1, 2, \ldots ,$$

$$n_{\text{max}} = \left\lceil \sqrt{A + \alpha(n - 1) + \alpha - 1} \right\rceil$$

and

for $\alpha > 1/2$

$$E_n = \frac{\hbar^2}{8\mu b^2} \left[ \frac{A + \alpha(n - 1)}{n + \alpha} - (n + \alpha) \right]^2,$$

$$n = 0, 1, 2, \ldots ,$$

$$n_{\text{max}} = \left\lceil \sqrt{A + \alpha(n - 1) - \alpha} \right\rceil$$

and

where $\varepsilon_n = \frac{1}{2} \left[ \frac{A + \alpha(n - 1)}{n - a + 1} - (n - \alpha + 1) \right].$

The normalization constants $N_n$ and $\bar{N}_n$ are calculated explicitly in the appendix. Note that $n_{\text{max}}$ is the number of bound states for the whole bound spectrum near the continuous zone. $n_{\text{max}}$ is the largest integer which is less than or equal to the value of $n$ that makes the right-hand side of equations (25) and (26) vanish. The above results are identical to equations (12) and (13) given in [34].

3. 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 $\alpha$. The results obtained by means of equation (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. Table 1 can be used to assess the validity and usefulness of our present approximations. The results of the energy spectrum for the 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 0.00075, 0.00087, 0.0014, 0.0017 and 0.011% for $n = 0, 1, 2, 3$ and $4$, respectively. However, when $1/b$ varies between 0.025 and 0.075, the range of accuracies can be 0.00075–0.0022%, 0.00087–0.068% and 0.0014–1.57% for $n = 0$ and $1$, respectively. In addition, we present the ro-vibrational energy states for a few diatomic molecules HCl, CH, LiH, CO, NO, O$_2$, I$_2$, N$_2$, H$_2$ and Ar; in tables 2–6. The lowest eigenvalues of $l = 0, 1, 2$ and 3 are given at four values of $1/b$ in the range 0.025–0.1 covering both weaker and stronger interactions to demonstrate the generality of

### Table 3. The ro-vibrational energy spectra ($-E_n$) (in eV) for LiH and CO for $2p$, $3p$, $3d$, $4p$, $4d$, $4f$, $5p$, $5d$, $5f$, $6p$, $6d$, $6f$ and $6g$ states with $\mu_{\text{LiH}} = 0.8801221$ amu, $\mu_{\text{CO}} = 0.8606719$ amu and $A = 2b$. 

| States | $1/b$ | LiH | CO |
|--------|--------|-----|-----|
|        | $\alpha = 0, 1$ | $\alpha = 0.75$ | $\alpha = 1.5$ | $\alpha = 0, 1$ | $\alpha = 0.75$ | $\alpha = 1.5$ |
| 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 | 0.547435 | 0.587664 | 0.429985 |
|        | 0.100  | 3.76057 | 4.04778 | 2.92374 | 0.482425 | 0.519270 | 0.375073 |
| 3p     | 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  | 0.94743 | 0.988358 | 0.815688 | 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 |
|        | 0.100  | 0.505009 | 0.520405 | 0.450139 | 0.064785 | 0.066760 | 0.057746 |
| 5p     | 0.025  | 0.942586 | 0.964223 | 0.864926 | 0.129920 | 0.126965 | 0.110957 |
|        | 0.050  | 0.935256 | 0.948967 | 0.884069 | 0.119979 | 0.121738 | 0.113413 |
|        | 0.075  | 0.475690 | 0.483161 | 0.444117 | 0.061024 | 0.062111 | 0.056974 |
|        | 0.100  | 0.105544 | 0.109984 | 0.089051 | 0.031540 | 0.031409 | 0.022424 |
| 5f     | 0.025  | 0.446540 | 0.465751 | 0.383735 | 0.057284 | 0.059749 | 0.049227 |
|        | 0.050  | 0.441654 | 0.451655 | 0.405420 | 0.056658 | 0.057941 | 0.052009 |
|        | 0.075  | 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 |
|        | 0.050  | 0.197105 | 0.206782 | 0.165379 | 0.025286 | 0.026527 | 0.021216 |
|        | 0.100  | 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 |
|        | 0.050  | 0.175116 | 0.177085 | 0.167554 | 0.022465 | 0.022717 | 0.021495 |

The units of $(\varepsilon_n - \varepsilon_{n'})$ are in pm.
Our results. The formalism is quite simple, computationally efficient, reliable and illustrated very accurately.

4. 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]

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

where \( Z \varepsilon^2 \) is the strength, \( \delta \) is the screening parameter and \( b \) is the range of the potential. If the potential is used for atoms, the \( Z \) is identified with the atomic number. Furthermore, taking \( b = 1/\delta \) and identifying \((A \hbar^2 / 2 \mu b^2)\) as \( Z \varepsilon^2 \delta \), we are able to obtain the ro-vibrating energy spectra and the normalized wave functions deduced from equations (19) and (24), respectively:

\[
E_{nl}(r) = N_{nl}e^{-\epsilon_{nl}/b}r \left( 1 - e^{-\epsilon_{nl}/b} \right)^{2} \times 2 F_1(-n, n + 2\epsilon_{nl} + v_l; 2\epsilon_{nl} + 1; e^{-\epsilon_{nl}/b}),
\]

\[
\epsilon_{nl} = \sqrt{\frac{2\mu E_{nl} + l(l + 1)D_0}{\hbar^2 \delta^2}} > 0,
\]

where \( N_{nl} \) is as given in the appendix. Also, for s-wave \((l = 0)\) states, we obtain

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

and

\[
E_{nl}(r) = N_{nl}e^{-\epsilon_{nl}/b}r \left( 1 - e^{-\epsilon_{nl}/b} \right)^{2} \times 2 F_1(-n, n + 2\epsilon_{nl} + v_l; 2\epsilon_{nl} + 1; e^{-\epsilon_{nl}/b}),
\]

\[
\epsilon_{nl} = \sqrt{\frac{2\mu E_{nl} + l(l + 1)D_0}{\hbar^2 \delta^2}} > 0,
\]

where \( N_{nl} \) can be easily found from either relation (A.7) or (A.9) after setting \( \alpha = 0 \) or \( \alpha = 1 \) in the appendix.
Table 5. The ro-vibrational energy spectra \((-E_{nl})\) (in eV) for I₂ and N₂ for 2p, 3p, 3d, 4p, 4d, 4f, 5p, 5d, 5f, 6p, 6d, 6f and 6g states with \(\mu_{\text{I}_2} = 63.452 235 02\text{ amu}, \mu_{\text{N}_2} = 7.003 35\text{ amu}\) and \(A = 2b\).

| States | 1/b | \(\alpha = 0, 1\) | \(\alpha = 0.75\) | \(\alpha = 1.5\) | \(\alpha = 0, 1\) | \(\alpha = 0.75\) | \(\alpha = 1.5\) |
|--------|-----|------------------|------------------|------------------|------------------|------------------|------------------|
| 2p     | 0.025 | 0.074 2866 | 0.079 4033 | 0.059 2729 | 0.673 056 | 0.719 416 | 0.537 028 |
|        | 0.050 | 0.066 5676 | 0.071 9350 | 0.052 7310 | 0.603 120 | 0.645 934 | 0.477 757 |
|        | 0.075 | 0.059 1925 | 0.063 5403 | 0.046 4914 | 0.536 300 | 0.575 692 | 0.421 225 |
| 3p     | 0.100 | 0.052 1615 | 0.056 1452 | 0.040 5541 | 0.472 597 | 0.508 691 | 0.367 431 |
|        | 0.125 | 0.050 1244 | 0.056 2500 | 0.034 5109 | 0.419 723 | 0.456 919 | 0.315 539 |
| 3d     | 0.075 | 0.157 5899 | 0.016 8309 | 0.012 4658 | 0.142 780 | 0.152 493 | 0.112 943 |
| 4p     | 0.100 | 0.100 5292 | 0.011 4221 | 0.007 8274 | 0.095 397 | 0.103 488 | 0.070 918 |
| 4d     | 0.025 | 0.079 2648 | 0.029 4980 | 0.026 0094 | 0.260 269 | 0.267 260 | 0.235 652 |
|        | 0.050 | 0.021 5761 | 0.022 1955 | 0.019 3987 | 0.195 485 | 0.201 097 | 0.175 757 |
|        | 0.075 | 0.015 4189 | 0.015 6319 | 0.013 4547 | 0.137 253 | 0.141 629 | 0.121 903 |
| 5p     | 0.100 | 0.009 4448 | 0.009 8072 | 0.008 1775 | 0.085 572 | 0.088 855 | 0.074 090 |
|        | 0.125 | 0.007 0794 | 0.011 7091 | 0.011 3138 | 0.119 070 | 0.124 209 | 0.102 506 |
| 5d     | 0.075 | 0.002 9890 | 0.003 3034 | 0.002 0323 | 0.027 081 | 0.029 930 | 0.018 413 |
| 5f     | 0.100 | 0.007 0488 | 0.007 2183 | 0.006 2437 | 0.063 465 | 0.065 400 | 0.056 570 |
| 5g     | 0.125 | 0.002 3790 | 0.002 5138 | 0.001 9052 | 0.021 554 | 0.022 776 | 0.017 261 |
| 6p     | 0.025 | 0.012 9726 | 0.013 1628 | 0.012 2626 | 0.117 535 | 0.119 258 | 0.111 102 |
| 6q     | 0.050 | 0.012 6785 | 0.010 6785 | 0.010 0785 | 0.059 781 | 0.060 845 | 0.055 813 |
| 6f     | 0.075 | 0.008 9850 | 0.010 0826 | 0.009 3250 | 0.111 264 | 0.136 240 | 0.111 122 |
| 6g     | 0.100 | 0.002 3790 | 0.002 5138 | 0.001 9052 | 0.021 554 | 0.022 776 | 0.017 261 |

\(2\beta = \) in pm.

respectively. Here, in this case \(v_n = v_n'\), and the number of bound states \(n_{\text{max}}\) is also the same in both relations (A.8) and (A.10). In the usual approximation [19] where \(D_0 = 0\) and \(D_1 = D_2 = 1\), equations (28) and (29) become

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

\[ 0 \leq n, l < \infty, \]

(32)

and

\[ u_{nl}(r) = N_{nl} e^{-\epsilon_{nl}/b} \left( 1 - e^{-r/b} \right)^{l+1} \]

\times \sqrt{2} F_1 \left( -n, n + 2 \left( \epsilon_{nl} + l + 1 \right); 2\epsilon_{nl} + 1; e^{-r/b} \right),

\[ \epsilon_{nl} = \sqrt{\frac{2\mu E_{nl}}{\hbar^2 \delta^2} > 0}, \]

(33)

where \(N_{nl}\) can be found from relation (A.6) by setting \(v_l = l + 1\). Essentially, these results coincide with those obtained by the Feynman integral method [17] and the standard way [18, 19]. Following [27] by taking \(D_1 = D_2 = 1\) and \(D_0 = 1/12\), equations (28) and (29) become

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

\[ + \frac{l(l+1)h^2 \delta^2}{24\mu}, \quad 0 \leq n, l < \infty, \]

(34)

\[ \epsilon_0 = \frac{Ze^2 h^2}{2\mu a_0}, \quad a_0 = \frac{h^2}{\mu e^2}, \]

(36)

which coincide, for the ground state, with equation (6) in Gönlü and Zorba [9]. The Hulthén potential behaves like the Coulomb potential near the origin \((r \to 0)\), 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. \(r/b < 1\)), the Hulthén potential becomes the Coulomb potential given by \(V_C(r) = -Ze^2/r\) with energy levels and wave functions

\[ E_{nl} = -\frac{\epsilon_0}{(n+l+1)^2}, \quad n, l = 0, 1, 2, \ldots, \]

\[ \psi_{nl}(r) = \frac{1}{r} e^{-r/b} \left( 1 - e^{-r/b} \right)^{l+1} \]

\[ \times \sqrt{2 \mu E_{nl} / \hbar^2 \delta^2} \left( -n, n + 2 \left( \epsilon_{nl} + l + 1 \right); 2\epsilon_{nl} + 1; e^{-r/b} \right), \]

\[ \epsilon_{nl} = \sqrt{\frac{2\mu E_{nl}}{\hbar^2 \delta^2} > 0}, \]

(35)
Table 6. The ro-vibrational energy spectra (−E_a) (in eV) for H_2 and Ar_2 for 2p, 3p, 4p, 5p, 6p, 7p, 8p, 9p, 10p, and He_2 states with μ_{H_2} = 0.504 07 amu, μ_{Ar_2} = 19.9812 amu and A = 2b.

| States | 1/β | H_2 | Ar_2 |
|--------|-----|-----|------|
|        | α = 0.1 | α = 0.75 | α = 1.5 | α = 0.1 | α = 0.75 | α = 1.5 |
| 2p     | 0.025 | 9.351 18 | 9.995 28 | 7.461 26 | 0.235 904 | 0.252 153 | 0.188 227 |
| 3p     | 0.025 | 8.379 51 | 8.974 35 | 6.637 77 | 0.211 392 | 0.226 398 | 0.167 452 |
| 4p     | 0.025 | 7.451 14 | 7.998 44 | 5.852 33 | 0.187 972 | 0.201 778 | 0.147 638 |
| 5p     | 0.025 | 6.566 08 | 7.067 55 | 5.104 95 | 0.165 644 | 0.178 295 | 0.128 784 |
| 6p     | 0.025 | 5.686 07 | 6.087 64 | 4.358 22 | 0.143 043 | 0.155 937 | 0.109 368 |
| 7p     | 0.025 | 4.824 06 | 5.054 64 | 3.661 22 | 0.121 490 | 0.133 987 | 0.092 192 |
| 8p     | 0.025 | 3.984 05 | 4.088 64 | 2.994 22 | 0.100 937 | 0.113 987 | 0.076 576 |
| 9p     | 0.025 | 3.174 04 | 3.298 64 | 2.352 22 | 0.081 490 | 0.093 987 | 0.062 192 |
| 10p    | 0.025 | 2.394 03 | 2.528 64 | 1.750 22 | 0.063 490 | 0.075 987 | 0.048 776 |

where ε_0 = 13.6 eV and a_0 is the Bohr radius for the Hydrogen atom [3]. The wave functions also take the form

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

\[ \times r^{l+1} F_0(2l+1; n+2) \left( \frac{2 \mu Z e^2 r^2}{\hbar^2 (n+1)} \right) \]

which is found to be identical to [11, 13].

5. Conclusions

We have applied an alternative improved approximation scheme for the centrifugal potential \( l(l+1)r^{-2} \) to obtain the energy levels and corresponding wave functions 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 \( 1/β \) 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 \( \alpha \) and \( l \). The precision of the resulting approximation of wave functions (24) for \( V_{nl}(r) \) in equation (5b) is due to the approximative character of the centrifugal term \( 1/r^2 \) in equation (6a) for \( l \neq 0 \) states because the wave functions are relevant to the bound-state energy approximation in equation (19). The approximation (6a) for the centrifugal potential allows us to obtain analytic approximations (34) and (35) for the eigenvalues and 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 equation (24)) because the correct (exact) wave functions, \( u_{nl}^{\text{exact}}(r) \), are still not found. Hence, the notation residual can be used for \( R = H_n^{\text{approx}} - E_n^{\text{approx}} \) of equations (5), are still not found. Hence, the notation residual can be used for \( R = H_n^{\text{approx}} - E_n^{\text{approx}} \) and the error (or deviation) for the difference \( u_{nl}^{\text{approx}}(r) - u_{nl}^{\text{exact}}(r) \). Due to the slowness of the numerical calculation of the hypergeometric functions \( F_0(-n, n + 2; \alpha; r) \) and their derivatives in Mathematica, the residual \( R \) is not evaluated. This residual is expected to be six orders of magnitude smaller than typical values \( E_n^{\text{approx}} \). Consequently, the error \( u_{nl}^{\text{approx}}(r) - u_{nl}^{\text{exact}}(r) \) is also expected to be small. Furthermore, the error in approximation of the Hamiltonian (4) with potential (5) is already small, since the approximation used in (6a) is valid only when \( r \ll b \) (small screening parameter \( \delta = 1/b \)). To demonstrate this, the NU results have been compared with the results of numerical integration procedures using a Mathematica program [28] and the results obtained from usual approximation schemes of the centrifugal potential [26]. For small \( 1/β \) values, the NU results are in good agreement with the ones obtained in [28], but in the high-screening region (large \( 1/β \)) 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 \( I = 0, \ l \neq 0 \) and the Hulthén potential. As we have seen, the NU method puts no constraint on the potential parameter values involved and is easy to implement. Our results are sufficiently accurate for practical purposes. Therefore, we have applied the present solution in equation (19) to obtain the ro-vibrational energies \((-E_{nl})\) for the HCl, CH, LiH, CO, NO, O₂, I₂, N₂, H₂ and Ar₂ diatomic molecules.

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Appendix. 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]), namely

\[
3F_1\left(-n, n + v + \mu + 1; v + 1; \frac{1 - x}{2}\right) = \frac{n!}{(v + 1)_n} P_n^{(v, \mu)}(x), (v + 1)_n = \frac{\Gamma(v + n + 1)}{\Gamma(v)}.
\]

(A.1)

to rewrite the wave functions in (24) as

\[
u_{nl}(r) = \mathcal{N}_{nl} n! (2n + 1) \left(2n + 1\right)^{-1/2} e^{-\alpha r/b} \times \left(1 - e^{-r/b}\right)^{n+1} P_n^{(2n+1, -1)}(1 - 2e^{-r/b}).
\]

(A.2)

From the normalization condition \( \int_{0}^{\infty} |\nu_{nl}(r)|^2 \, dr = 1 \) and under the coordinate change \( x = 1 - 2e^{-r/b} \), the normalization constant in (A.2) is given by

\[
\mathcal{N}_{nl}^{-2} = b \left[\frac{n! (2n + 1)}{\Gamma(n + 2n + 1)}\right]^2 \left[\frac{1 - x}{2}\right]^{2n+1} \times \left[\frac{1 + x}{2}\right]^{2n} \left[\frac{2n+1}{2}\right] \left[\frac{1 + x}{2}\right]^{2n} \left[\frac{1 + x}{2}\right]^{2n+1} P_n^{(2n, 2n+1)}(x)^2 \, dx.
\]

(A.3)

The calculation of this integral can be performed by writing

\[
\frac{1 + x}{2} = 1 - \left(\frac{1 - x}{2}\right)
\]

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

\[
\int_{-1}^{1} (1 - x)^{v-1} (1 + x)^{\mu} \left[\frac{P_n^{(\nu, \mu)}(x)}{n! \Gamma(n + \mu + 1)}\right]^2 \, dx
\]

\[
= 2^{\nu+\mu} \frac{(n + v + 1) \Gamma(n + \mu + 1)}{n! \Gamma(n + \nu + \mu + 1)},
\]

(A.4)

which is valid for \( \Re(\nu) > 0 \) and \( \Re(\mu) > -1 \), and (see formula (7.391.1) in [35])

\[
\int_{-1}^{1} (1 - x)^v (1 + x)^\mu \left[\frac{P_n^{(\nu, \mu)}(x)}{n! \Gamma(n + \mu + 1)}\right]^2 \, dx
\]

\[
= 2^{\nu+\mu+1} \frac{\Gamma(n + v + 1) \Gamma(n + \mu + 1)}{n! \Gamma(n + v + \mu + 1) (2n + v + \mu + 1)},
\]

(A.5)

which is valid for \( \Re(\nu) > -1, \Re(\mu) > -1 \). This leads to

\[
\mathcal{N}_{nl} = \frac{1}{\Gamma(2n + 1)} \left[\frac{\epsilon_n (n + \nu + \mu + 1)}{2b (n + v + \mu)}\right]
\]

\[
\times \frac{\Gamma((n + 2\nu) - 1) \Gamma(n + 2\nu + 2\mu)}{n! \Gamma(n + 2\mu + 1)}\right]^{1/2},
\]

(A.6)

where \( 0 < n < n_{\text{max}} = \frac{\sqrt{A + \alpha (\alpha - 1)} - \alpha}{2(\alpha - 2)} \). in the case of the s-wave (\( l = 0 \) case), the above result is written explicitly as follows:

\[
\mathcal{N}_{nl} = \frac{1}{\Gamma(2n + 1)} \left[\frac{\epsilon_n (n + \nu + \mu + 1)}{2b (n + v + \mu)}\right]
\]

\[
\times \frac{\Gamma((n + 2\nu) - 1) \Gamma(n + 2\nu + 2\mu)}{n! \Gamma(n + 2\mu + 1)}\right]^{1/2},
\]

(A.7)

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

\[
\mathcal{N}_{nl} = \frac{1}{\Gamma(2n + 1)} \left[\frac{\epsilon_n (n + \nu + \mu + 1)}{2b (n + v + \mu)}\right]
\]

\[
\times \frac{\Gamma((n + 2\nu) + 1) \Gamma((n + 2\nu + 2\mu) + 2\alpha)}{n! \Gamma(n + 2\mu + 2\alpha)}\right]^{1/2},
\]

(A.9)

where

\[
\epsilon_n = \frac{A + \alpha (\alpha - 1)}{2(\alpha - 1)} - \frac{n - \alpha + 1}{2},
\]

(A.8)

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

\[
\epsilon_n = \frac{A + \alpha (\alpha - 1)}{2(\alpha - 1)} - \frac{n - \alpha + 1}{2},
\]

(A.10)

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

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