

Approximate analytical solutions of a two-term diatomic molecular potential with centrifugal barrier

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Abstract Approximate analytical bound state solutions of the radial Schrödinger equation are studied for a two-term diatomic molecular potential in terms of the hypergeometric functions for the cases where $q \geq 1$ and $q = 0$. The energy eigenvalues and the corresponding normalized wave functions of the Manning–Rosen potential, the ‘standard’ Hulthén potential and the generalized Morse potential are briefly studied as special cases. It is observed that our analytical results are the same with the ones obtained before.

Keywords Diatomic molecular potential · Schrödinger equation · Bound state

1 Introduction

In this letter, we study the bound state solutions of a diatomic molecular potential having the form

$$V(r, \beta, q) = -V_0 \frac{e^{-\beta r}}{1 - qe^{-\beta r}} + V_1 \frac{e^{-2\beta r}}{(1 - qe^{-\beta r})^2}, \quad (1)$$

which has been firstly presented by Sun to fit some experimental data of some diatomic molecular systems [1]. Analytical studying of the above potential could be interesting since it involves several potential forms (for example, $q = 0$ gives the Morse potential,

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$q > 0$ corresponds to the ‘generalized’ Hulthén potential, *etc.*) meaning that we can simply extend the solutions to the ones of these special cases.

The above potential is one of the central potentials which are a powerful ground for experimental and theoretical computations in different areas of physics such as in high energy physics where they were used to describe hadrons as bound states [2] in atomic physics where some important subjects such as binding energy and inclusive momentum distributions are studied by using of central potentials [3], in theoretical molecular dynamics model to study the intramolecular and intermolecular interactions and atomic pair correlation functions [4]. Moreover, the central potentials have been used in an important quantum mechanical problem which is also related with quantum information theory, the Fisher uncertainty relation and applied to the hydrogen atom and isotropic harmonic oscillator [5] and also for some theoretical calculations within the information theory to study some statistical quantities such as the Boltzmann-Shannon entropy [6]. The construction of an algorithm could be an interesting problem where the aim is to solve the radial Schrödinger equation (SE) for a given central potential $V(r)$ numerically [7].

To our knowledge, the potential under consideration has been studied within the supersymmetric quantum mechanics [8] and in terms of Green’s function [9] in non-relativistic domain. We search the bound state spectrum and the wave functions of the above potential by using an approximation instead of the centrifugal term in the same domain. We find an analytical expression for the energy spectrum and obtain the normalization constant by using some properties of the hypergeometric functions. Throughout this work, we restrict ourself to the cases where $q \geq 1$ and $q = 0$ and give our numerical results for two diatomic molecules for different values of quantum number pair (n, ℓ) .

2 Energy spectrum and wave functions

The radial Schrödinger equation is written [10]

$$\frac{d^2 R(r)}{dr^2} + \left\{ \frac{2m}{\hbar^2} [E_{n\ell} - V(r)] - \frac{\ell(\ell + 1)}{r^2} \right\} R(r) = 0, \quad (2)$$

where ℓ is the angular momentum quantum number, m is the particle mass, $V(r)$ is the central potential and $E_{n\ell}$ is the non-relativistic energy. Inserting Eq. (1) into Eq. (2) gives

$$\frac{d^2 R(r)}{dr^2} + \left\{ -\frac{2mV_1}{\hbar^2} \frac{1}{(e^{\beta r} - q)^2} + \frac{2mV_0}{\hbar^2} \frac{1}{e^{\beta r} - q} + \frac{2mE_{n\ell}}{\hbar^2} - \frac{\ell(\ell + 1)}{r^2} \right\} R(r) = 0. \quad (3)$$

where V_0, V_1, β and q are real parameters defined by $V_1 = D_0(e^\mu - q)$, $V_0 = 2V_1$, $\beta = \mu/r_0$, where D_0 is the depth of the potential, r_0 is the equilibrium of the molecule and q is the shape parameter.

We use the following approximation [11] instead of the centrifugal term among the others [12–15] to obtain an analytical solution of Eq. (3)

$$\frac{1}{r^2} \approx \beta^2 \frac{e^{\beta r}}{(e^{\beta r} - q)^2}, \quad (4)$$

Defining a new variable $z = qe^{-\beta r}$ and taking a trial function as $R(z) = z^{A_1}(1 - z)^{A_2}\phi(z)$ and with the help of Eq. (4), Eq. (3) turns into

$$z(1 - z) \frac{d^2\phi(z)}{dz^2} + [1 + 2A_1 - (1 + 2A_1 + 2A_2)z] \frac{d\phi(z)}{dz} + \left\{ -2A_1A_2 - A_2^2 + \frac{2mV_1}{\beta^2\hbar^2} + \frac{2mV_0}{q\beta^2\hbar^2} \right\} \phi(z) = 0, \quad (5)$$

where we set the parameters

$$A_1^2 = -\frac{2mE_n\ell}{\hbar^2}, \quad (6a)$$

$$A_2(A_2 - 1) = \frac{1}{q} \ell(\ell + 1) + \frac{2mV_1}{\beta^2\hbar^2}. \quad (6b)$$

By using the abbreviations

$$c = 1 + 2A_1, \quad (7a)$$

$$b = A_1 + A_2 + \sqrt{A_1^2 + \frac{2m}{\beta^2\hbar^2} \left(V_1 + \frac{V_0}{q} \right)}, \quad (7b)$$

$$a = A_1 + A_2 - \sqrt{A_1^2 + \frac{2m}{\beta^2\hbar^2} \left(V_1 + \frac{V_0}{q} \right)}, \quad (7c)$$

Equation (5) becomes an equation having the form of the hypergeometric-type equation [16]

$$z(1 - z)\phi''(z) + [c - (a + b + 1)z]\phi'(z) - ab\phi(z) = 0, \quad (8)$$

whose solution is the hypergeometric functions

$$\phi(z) \sim {}_2F_1(a, b; c; z). \quad (9)$$

When either a or b equals to a negative integer $-n$, the hypergeometric function $\phi(z)$ can be reduced to a finite solution. This gives us a polynomial of degree n in Eq. (9) and the following quantum condition

$$A_1 + A_2 - \sqrt{A_1^2 + \frac{2m}{\beta^2\hbar^2} \left(V_1 + \frac{V_0}{q} \right)} = -n, \quad (10)$$

Table 1 Energy eigenvalues of the H_2 molecule in eV ($E_{n\ell} < 0$)

n	ℓ	$q = 1.25$	$q = 1.50$	$q = 1.75$
0	0	3.8099200	2.3409000	1.5021100
1	0	2.6465800	1.4911800	0.8623870
	1	2.6295900	1.4804000	0.8551840
2	0	1.7526700	0.8721010	0.4265830
	1	1.7394900	0.8642480	0.4217640
	2	1.7133000	0.8486670	0.4122170
3	0	1.0823900	0.4428370	0.1570130
	1	1.0724800	0.4374880	0.1542230
	2	1.0528200	0.4269000	0.1487240
	3	1.0237200	0.4112900	0.1406770
4	0	0.5991580	0.1711030	0.0242272
	1	0.5920830	0.1679170	0.0231832
	2	0.5780760	0.1616440	0.0211659
	3	0.5574210	0.1524740	0.0183168
	4	0.5305400	0.1406920	0.0148458
5	0	0.2734990	0.0311495	0.0049878
	1	0.2689040	0.0298494	0.0054591
	2	0.2598410	0.0273349	0.0064646
	3	0.2465630	0.0237765	0.0081293
	4	0.2294460	0.0194276	0.0106393
	5	0.2089850	0.0146225	0.0142399

which gives the energy values of the two-term potential for any ℓ -values

$$E_{n\ell} = -\frac{\beta^2 \hbar^2}{2m} \left\{ \frac{n^2 + (2n + 1) \left(A'_2 + \frac{1}{2} \right) + \frac{1}{q} \left[\ell(\ell + 1) - \frac{2mV_0}{\beta^2 \hbar^2} \right]}{2n + 1 + 2A'_2} \right\}^2, \quad (11)$$

where

$$A'_2 = \sqrt{\frac{1}{4} + \frac{\ell(\ell + 1)}{q} + \frac{2mV_1}{\beta^2 \hbar^2}}. \quad (12)$$

By using Eq. (10) we obtain the total wave functions

$$R(z) = Nz^{A_1}(1 - z)^{A_2} {}_2F_1(-n, n + 2A_1 + 2A_2; 1 + 2A_1; z). \quad (13)$$

where N is the normalization constant and will be derived in Appendix A.

We summarize our numerical results in Tables 1 and 2 where the computations are made for two diatomic molecules, namely H_2 and LiH . The values of potential

Table 2 Energy eigenvalues of the *LiH* molecule in eV ($E_{n\ell} < 0$)

n	ℓ	$q = 1.25$	$q = 1.50$	$q = 1.75$
0	0	3.5677900	2.3156300	1.5836900
1	0	3.0290300	1.9055500	1.2595300
	1	3.0250700	1.9029400	1.2577000
2	0	2.5506900	1.5476900	0.9820380
	1	2.5471400	1.5453900	0.9804600
	2	2.5400700	1.5408100	0.9773080
3	0	2.1274300	1.2372900	0.7468470
	1	2.1242700	1.2352900	0.7455040
	2	2.1179600	1.2312900	0.7428200
	3	2.1085100	1.2253000	0.7388050
4	0	1.7544800	0.9701380	0.5500770
	1	1.7516800	0.9684030	0.5489500
	2	1.7460700	0.9649380	0.5466990
	3	1.7376900	0.9597550	0.5433330
	4	1.7265600	0.9528690	0.5388640
5	0	1.4275700	0.7424420	0.3882750
	1	1.4251000	0.7409570	0.3873480
	2	1.4201500	0.7379920	0.3854990
	3	1.4127600	0.7335570	0.3827350
	4	1.4029300	0.7276680	0.3790660
	5	1.3907100	0.7203470	0.3745090

parameters we used for these molecules are as follows [13]: $D_0 = 4.744600$ eV, $r_0 = 0.741600$ Å, $m = 0.503910$ amu, $\mu = 1.440558$ and $E_0 = \hbar^2/(mr_0^2) = 1.508343932 \times 10^{-2}$ eV for H_2 molecule and $D_0 = 2.515287$ eV, $r_0 = 1.595600$ Å, $m = 0.8801221$ amu, $\mu = 1.7998368$ and $E_0 = 1.865528199 \times 10^{-3}$ eV for *LiH* molecule [17]. It is seen that the energy values decrease while the values of the quantum numbers increase and the energy eigenvalues are also inversely proportional with the shape parameter for each of the molecules.

Now we intend briefly to study some special cases whose energy eigenvalue equation obtained from Eq. (11) by suitable choices of the potential parameters.

2.1 Manning–Rosen potential

The Manning–Rosen potential can be written as [18]

$$V(r) = -\frac{A\hbar^2}{2mb^2} \frac{1}{e^{r/b} - 1} + \frac{\alpha(\alpha - 1)\hbar^2}{2mb^2} \frac{1}{(e^{r/b} - 1)^2}, \quad (14)$$

Table 3 Energy eigenvalues obtained from Eqs. (15), (18) and (30)

Manning–Rosen potential				
n	ℓ	$1/b$	Present work	Ref. [19]
2	1	0.025	-0.1205793	-0.1205279
		0.050	-0.1084228	-0.1082170
		0.075	-0.0969120	-0.0964490
		0.100	-0.0860470	-0.0852240
Hulthén potential				
n	ℓ	δ	Present work	Ref. [21]
0	1	0.025	-0.1128130	-0.1127600
		0.050	-0.1012500	-0.1010420
		0.075	-0.0903120	-0.0898450
		0.100	-0.0800000	-0.0791700
		0.150	-0.0612500	-0.0594950
Morse potential				
n			Present work	Ref. [17]
0			-4.476013	-4.476013
1			-3.962315	-3.962315
2			-3.479919	-3.479918
3			-3.028824	-3.028823
4			-2.609030	-2.609029
5			-2.220537	-2.220536

If we write our parameters as $V_0 = \frac{A}{2b^2}$; $V_1 = \frac{\alpha(\alpha-1)}{2b^2}$; $\beta = \frac{1}{b}$ and $q = 1$ then we obtain the energy eigenvalues of the Manning–Rosen potential

$$E_{n\ell} = -\frac{1}{2b^2} \left\{ \frac{n^2 + (2n + 1) \left(\frac{1}{2} + \sqrt{\frac{1}{4} + \ell(\ell + 1) + \alpha(\alpha - 1)} \right) + \ell(\ell + 1) - A}{2n + 1 + 2\sqrt{\frac{1}{4} + \ell(\ell + 1) + \alpha(\alpha - 1)}} \right\}^2 \quad (15)$$

which is the same result obtained in Ref. [19]. The normalization constant in Eq. (13) is obtained from Eq. (A8) as

$$N = \left\{ \frac{1}{g(A_1^{(1)}, A_2^{(1)}, k)g(A_1^{(1)}, A_2^{(1)}, l) {}_2F_1(-2A_2^{(1)}, 1 + 2A_1^{(1)} + k + l; 2 + 2A_2^{(1)} + k + l; 1)} \right\}^{1/2} \quad (16)$$

where $A_1^{(1)} = \sqrt{-2mE_{n\ell}b^2/\hbar^2}$ and $A_2^{(1)} = (1/2)(1 + \sqrt{1 + 4\ell(\ell + 1) + 4m\alpha(\alpha - 1)/\hbar^2})$.

We summarize our numerical results obtained from Eq. (15) in Table 3 where we set the parameters as $A = 2b$ and $\alpha = 0.75$ to compare the results with the ones given in Ref. [19]. Please note that the parameter D_0 used in Ref. [19] is zero in the present

work since our approximation used for the centrifugal term is different from the one used in Ref. [19] where energy eigenvalues are computed in atomic units.

2.2 Standard Hulthén potential

Equation (1) gives the standard Hulthén potential for $V_1 = 0$ and $q = 1$

$$V(r) = -V_0 \frac{e^{-\beta r}}{1 - e^{-\beta r}}, \quad (17)$$

and we obtain the energy eigenvalues from Eq. (11)

$$E_{n\ell} = -\frac{\beta^2 \hbar^2}{2m} \left\{ \frac{(n + \ell)(n + \ell + 2) + 1 - \frac{2mV_0}{\beta^2 \hbar^2}}{2(n + 1 + \ell)} \right\}^2. \quad (18)$$

and the normalization constant of the corresponding wave functions from Eq. (A8)

$$N = \left\{ \frac{\Gamma(2 + 4A_2^{(2)} + k + \ell)}{g(A_1, A_2^{(2)}, k)g(A_1, A_2^{(2)}, \ell)(1 + 2A_2^{(2)} + k + \ell)\Gamma(1 - 2A_1 + 4A_2^{(2)})} \right\}^{1/2} \quad (19)$$

where $A_2^{(2)} = 1 + \ell$. Choosing the parameters as $\beta = \frac{1}{a}$ and $V_0 = \alpha$ gives the following expression ($m = \hbar = 1$)

$$E_{n\ell} = -\frac{1}{2a^2} \left\{ \frac{(n + \ell)(n + \ell + 2) + 1 - 2\alpha a^2}{2(n + 1 + \ell)} \right\}^2. \quad (20)$$

which is the same result given in Ref. [20]. The standard Hulthén potential in Eq. (16) could give the Coulomb potential for $\beta r \ll 1$

$$V(r) = -\frac{Ze^2}{r}, \quad (21)$$

where we set $V_0 = Ze^2\beta$. We obtain the energy spectrum of the Coulomb potential from Eq. (18) ($m = \hbar = e = 1$)

$$E_{n\ell} = -\frac{Z^2}{2(n + 1 + \ell)^2}. \quad (22)$$

which is the same result obtained in Ref. [19]. The normalization constant of the corresponding wave functions is given with the help of Eq. (19) under the above assumptions.

The numerical energy values of the Hulthén potential obtained from Eq. (18) are placed in second part of Table 3 for different quantum number pair (n, ℓ) in atomic units. We choose the parameters as $V_0 = \beta = \delta$ as in Ref [21].

2.3 Generalized Morse potential

We obtain the generalized Morse potential for the limit $q \rightarrow 0$ in Eq. (1)

$$V(r) = V_1 e^{-2\beta r} - V_0 e^{-\beta r}, \tag{23}$$

which gives the following equation for s -waves

$$\left(\frac{d^2}{dr^2} + \frac{2mV_1}{\hbar^2} e^{-\beta r} - \frac{2mV_0}{\hbar^2} e^{-2\beta r} + \frac{2mE_{n\ell}}{\hbar^2} \right) R(r) = 0, \tag{24}$$

Defining a new variable $z = e^{-\beta r}$ and taking the wave function of the form $R(z) = e^{-B_1 z/2} z^{B_2/2} \phi(z)$ we obtain

$$z \frac{d^2 \phi(z)}{dz^2} + \left(1 + \frac{B_2}{2} - B_1 z \right) \frac{d\phi(z)}{dz} + \left\{ -\frac{B_1 B_2}{2} - \frac{B_1}{2} + \frac{2mV_1}{\beta^2 \hbar^2} \right\} \phi(z) = 0, \tag{25}$$

where $B_1^2 = \frac{8mV_0}{\beta^2 \hbar^2}$ and $B_2^2 = \frac{8mE}{\beta^2 \hbar^2}$. Using a new variable $y = B_1 z$ gives

$$y \frac{d^2 \phi(y)}{dy^2} + \left(1 + \frac{B_2}{2} - y \right) \frac{d\phi(y)}{dy} + \left\{ -\frac{B_2}{2} - \frac{1}{2} + \frac{2mV_1}{B_1 \beta^2 \hbar^2} \right\} \phi(y) = 0, \tag{26}$$

which is the Laguerre differential equation

$$xy'' + (\alpha + 1 - y)y' + ny = 0. \tag{27}$$

where the factor n should be zero or a positive integer to get a polynomial solution [22]. So, the solution of Eq. (25) are given in terms of the Laguerre polynomials as

$$\phi(y) \sim L_n^{\bar{\sigma}}(y), \tag{28}$$

where $\bar{\sigma} = B_2/2$ and $n = -\frac{B_2}{2} - \frac{1}{2} + \frac{2mV_1}{B_1 \beta^2 \hbar^2}$. We get the total eigenfunctions of the Morse potential

$$R(z) = N e^{-B_1 z/2} z^{B_2/2} L_n^{\bar{\sigma}}(B_1 z). \tag{29}$$

and the energy eigenvalues

$$E_{n\ell} = -\frac{\beta^2 \hbar^2}{8m} \left\{ 2n + 1 - \frac{V_1}{\beta \hbar} \sqrt{\frac{2m}{V_0}} \right\}^2. \tag{30}$$

We present the numerical energy values of the Morse potential obtained from the above equation in Table 3. We give the results for H_2 molecule (in eV) by taking the same

parameter values to obtain the results given in Table 1 and by setting the potential parameters as $V_0 = 2D_0$, $V_1 = D_0$.

Using the following representation of the Laguerre polynomials [22]

$$L_n^{\bar{\sigma}}(x) = \sum_{k=0}^n (-1)^k \binom{n + \bar{\sigma}}{n - k} \frac{x^k}{k!}, \quad (31)$$

the normalization condition is written as

$$|N|^2 g(n)g(m) \int_0^1 e^{B_1 z} z^{B_2+2k} dz = 1, \quad (32)$$

where

$$g(n) = \sum_{k=0}^n (-1)^k \binom{n + \frac{B_2}{2}}{n - k} \frac{B_1^k}{k!}; \quad g(m) = \sum_{k=0}^m (-1)^k \binom{m + \frac{B_2}{2}}{m - k} \frac{B_1^k}{k!}. \quad (33)$$

Changing the variable $t = B_1 z$ in Eq. (32) gives

$$|N|^2 g(n)g(m) B_1^{-(1+B_2+2k)} \int_0^1 e^{-t} t^{B_2+2k} dt = 1, \quad (34)$$

which includes the incomplete Gamma function defined as [21]

$$\gamma(a, x) \equiv \int_0^x t^{a-1} e^{-t} dt = \frac{1}{a} x^a e^{-x} {}_1F_1(1; 1 + a; x), \quad (35)$$

Finally the normalization constant is obtained as

$$N = \left\{ \frac{e\Omega B_1^\Omega}{g(n)g(m) {}_1F_1(1; 1 + \Omega; 1)} \right\}^{1/2}, \quad \Omega = 1 + B_2 + 2k. \quad (36)$$

3 Conclusion

We have studied the approximate bound state solutions of the radial SE equation for a two-term potential. We have obtained the energy eigenvalues and the corresponding normalized wave functions approximately in terms of the hypergeometric functions. We have presented our numerical results of the energy eigenvalues of two diatomic molecules in Tables 1 and 2. We have also studied the analytical bound state solutions of the Manning–Rosen potential, the ‘standard’ Hulthén potential and the generalized Morse potential as special cases. We have observed that our all analytical results are

the same with the ones obtained in the literature. We have also summarized some numerical results of the energy eigenvalues of the above three potentials in Table 3 and observed that our results are good agreement with the ones obtained before.

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Appendix A: Normalization constant

The wave functions in Eq. (13) is

$$R(z) = Nz^{A_1}(1 - z)^{A_2} {}_2F_1(-n, n + 2A_1 + 2A_2; 1 + 2A_1; z), \tag{A1}$$

which is written in terms of the new variable $z = q\xi$ ($0 \leq \xi \leq 1$)

$$R(q\xi) = Nq^{A_1}\xi^{A_1}(1 - q\xi)^{A_2} {}_2F_1(-n, n + 2A_1 + 2A_2; 1 + 2A_1; q\xi), \tag{A2}$$

The normalization condition $\int_0^1 |R(q\xi)|^2 d\xi = 1$ gives

$$|N|^2 q^{1+2A_1} \int_0^1 \xi^{2A_1}(1 - q\xi)^{2A_2} [{}_2F_1(-n, n + 2A_1 + 2A_2; 1 + 2A_1; q\xi)]^2 dx = 1. \tag{A3}$$

Using the representation of the hypergeometric functions [22]

$${}_2F_1(-n, b; c; z) = \sum_{k=0}^n \frac{(-n)_k (b)_k}{(c)_k k!} z^k, \tag{A4}$$

Equation (A3) becomes

$$|N|^2 q^{1+2A_1} g(A_1, A_2, k)g(A_1, A_2, l) \int_0^1 \xi^{2A_1+k+l}(1 - q\xi)^{2A_2} d\xi = 1, \tag{A5}$$

where $(-n)_k = (-1)^k(n - k + 1)_k = (-1)^k \frac{\Gamma(n+1)}{\Gamma(n-k+1)}$ and

$$g(A_1, A_2, k) = \sum_{k=0}^n \frac{(-n)_k (n + 2A_1 + 2A_2)_k}{(1 + 2A_1)_k k!} z^k. \tag{A6}$$

and $g(A_1, A_2, l) = g(A_1, A_2, k \rightarrow l)$.

Using the following identity for the hypergeometric functions [22]

$${}_2F_1(\alpha', \beta'; \delta'; z) = \frac{\Gamma(\delta')}{\Gamma(\beta')\Gamma(\delta' - \beta')} \int_0^1 t^{\beta'-1} (1-t)^{\delta'-\beta'-1} (1-tz)^{-\alpha'} dt, \quad (\text{A7})$$

we obtain the normalization constant from Eq. (A5)

$$N = \left\{ \frac{1}{q^{1+2A_1} g(A_1, A_2, k) g(A_1, A_2, l) {}_2F_1(-2A_2, 1+2A_1+k+l; 2+2A_2+k+l; q)} \right\}^{1/2}. \quad (\text{A8})$$

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