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BOUND STATE SOLUTIONS TO THE SCHRÖDINGER EQUATION FOR SELECTED DIATOMIC MOLECULES

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Abstract

In this study, the solutions of the Schrödinger equation are obtained with a class of inversely quadratic plus Hulthén potential models using the Nikiforov-Uvarov method with an approximation to the centrifugal term. We obtained the energy eigenvalue equation and normalized wave function. The energy equation was used to compute the numerical bound state for selected diatomic molecules (N_2, O_2, NO, and CO) for different rotational and vibrational quantum numbers utilizing their corresponding spectroscopic data. Our findings demonstrate that the energy eigenvalues are highly sensitive to the potential and diatomic molecule characteristics, with no divergence between the l-wave and s -wave, implying that the approximation scheme is well suited for these set of potentials. We also found eight special cases of this potential, and the results are consistent with previous reports in the literature.

Keywords**:** Schrödinger equation; Nikiforov-Uvarov method; class of inversely quadratic plus Hulthén potential; Diatomic molecules

Introduction

The dynamics and interactions of non-relativistic spinless particles and quantum–mechanical processes can be studied by the use of the time-independent Schrödinger wave equation [1-4]. The analytical solutions to this equation with physical potentials presume a significant part in our knowledge of the fundamental basis of a quantum system; because the eigenvalues and eigenfunctions related to quantum problems contain vital information concerning the quantum system [5, 6]. Nevertheless, the bound state solutions of the Schrödinger equation of a number of these potentials are feasible for a few cases, for example, Coulomb potential [7], Woods-Saxon [8], Hulthén [9], Manning-Rosen [10], and others. Additionally, when the arbitrary angular momentum quantum number l is available, one can solve the Schrödinger equation approximately by utilizing a reasonable approximation scheme [11]. Some of such approximations include the approximation scheme proposed by Greene and Aldrich [11], the improved approximation scheme by Jia et al. [12], the approximation scheme by Hill [13], the Pekeris approximation [14], the approximation scheme by Yazarloo et al. [15], and upgraded approximation scheme in Ref.[16].

Over the years, different quantum mechanical procedures have been utilized comprehensively aiming to get the exact and approximate solutions to the Schrödinger equation [17-39]. Inversely quadratic Hellmann potential (IQHP) was instituted from Hellmann potential [40], which has been widely utilized by numerous authors to get the energy of the bound state in atomic, nuclear, and particle physics [41,42]. From that point forward, it has been used by numerous authors to acquire the energy-bound state in different areas of physics [43-46]. Another intriguing potential with regards to this investigation is inversely quadratic potential (IQP). The IQP has been used by Oyewumi and Bangudu [47] in a mix with an isotropic harmonic oscillator in N-dimension space. Since that time, several papers in blend with this potential have shown up in the literature [48-50].

The Hulthén potential [51] is fundamental in exploring the interaction existing between two particles. It is applied in areas of physics such as nuclear and molecular physics, atomic physics, condensed matter physics, and chemical physics [52, 53].

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The aim of this study is to obtain the approximate bound state analytical solutions to the Schrödinger equation with the class of inversely quadratic plus Hulthén potential (CIQHP). The potential is obtained by the superposition of IQHP plus IQP (collectively known as the class of inversely quadratic potential) plus Hulthén potential. This potential has its application where its components are useful. The essence of combining at least two potential models is to have a more extensive scope of utilizations [54, 55]. The class of inversely quadratic plus Hulthén potential is of the form:

$$V(r) = -\frac{V_0}{r} + \frac{V_2 e^{-\delta r}}{r^2} - \frac{V_1}{r^2} - \frac{V_3 e^{-\delta r}}{1-e^{-\delta r}}. \tag{1}$$

The shape of this potential as a function of the screening parameter is given in Fig. 1. The paper is organized as follows: In Sect. 2, we solve the Schrödinger equation with the CIQHP to obtain the energy eigenvalues and normalized eigenfunctions. In Sect. 3, the derived energy equation will be used to obtain the numerical computation of energy eigenvalues at different states of the selected diatomic molecules. In Sect. 4, we present the results of various plots and the discussion. Conclusions are given in Sect. 5.

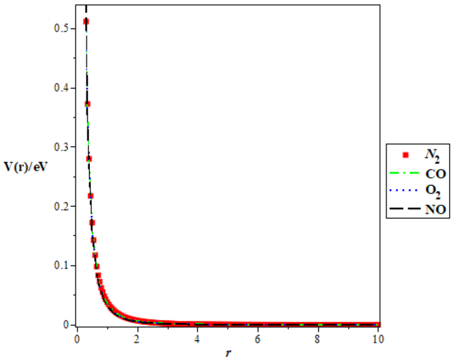

Fig. 1 Variation of the potential $V(r)$ against internuclear distance r for the N_2, O_2, NO and CO diatomic molecules

2. Approximate solution of Schrödinger equation with the class of inversely quadratic plus Hulthén potential

In this study, we adopt the Nikiforov-Uvarov method which is based on solving the second-order differential equation of the hypergeometric type. The details can be found in Ref. [17]. The Schrödinger equation of a quantum physical system is characterized by a given potential $V(r)$ reads [56]

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right)\psi_n(r) = E_n \psi_n(r), \tag{2}$$

where $\psi_n(r)$ is the eigenfunctions, E_n is the energy eigenvalues of the quantum system, n represents the set of all possible solutions, which determines a particular state of the quantum system, μ is the reduced mass of the system, $\hbar$ is the reduced Planck's constant and r is the radial distance from the origin. Substituting Eq. (1) into Eq. (2) gives

$$\frac{d^2\psi_n(r)}{dr^2} + \left[\frac{2\mu E_n}{\hbar^2} + \frac{2\mu V_0}{\hbar^2 r} - \frac{2\mu V_1 e^{-\delta r}}{\hbar^2 r^2} + \frac{2\mu V_2}{\hbar^2 r^2} + \frac{2\mu V_3 e^{-\delta r}}{\hbar^2\left(1-e^{-\delta r}\right)} - \frac{l(l+1)}{r^2}\right]\psi_n(r) = 0 \tag{3}$$

Equation (3) cannot be solved exactly with the proposed potential. So we introduce the Greene-Aldrich approximation scheme [57] to deal with the centrifugal barrier. This approximation scheme is a good approximation to the centrifugal term which is valid for $\delta << 1$, and it becomes

$$\frac{1}{r^2} \approx \frac{\delta^2}{\left(1-e^{-\delta r}\right)^2}. \tag{4}$$

Applying the approximation scheme in Eq. (5), one can obtain

$$\frac{d^2\psi_n(x)}{dx^2} + \left[\frac{2\mu E_n}{\hbar^2} + \frac{2\mu V_0 \delta}{\hbar^2\left(1-e^{-\delta r}\right)} - \frac{2\mu V_1 \delta^2 e^{-\delta r}}{\hbar^2\left(1-e^{-\delta r}\right)^2} + \frac{2\mu V_2 \delta^2}{\hbar^2\left(1-e^{-\delta r}\right)^2} + \frac{2\mu V_3 e^{-\delta r}}{\hbar^2\left(1-e^{-\delta r}\right)} - \frac{\delta^2 l(l+1)}{\left(1-e^{-\delta r}\right)^2}\right]\psi_n(x) = 0 \tag{5}$$

By using the change of variable from $r \longrightarrow x$, our new coordinate becomes

$$x = e^{-\delta r}. \tag{6}$$

We substitute Eq. (6) into Eq. (5) and after some simplifications, we have:

$$\frac{d^2\psi(x)}{dx^2}+\frac{1-x}{x(1-x)}\frac{d\psi(x)}{dx}+\frac{1}{\left[x(1-x)\right]^2}\left[-(\varepsilon+\beta_3)x^2+(2\varepsilon+\beta_0-\beta_1+\beta_3)x-(\varepsilon-\beta_0-\beta_2+\gamma)\right]\psi(x)=0, \tag{7}$$

where

$$\left.-\varepsilon=\frac{2mE_{nl}}{\delta^2\hbar^2},\quad \beta_0=\frac{2mV_0}{\delta\hbar^2},\quad \beta_1=\frac{2mV_1}{\hbar^2},\quad \beta_2=\frac{2mV_2}{\hbar^2},\quad \beta_3=\frac{2mV_3}{\delta^2\hbar^2},\quad \gamma=l(l+1)\right\}. \tag{8}$$

Comparing Eq. (7) and Eq. (1) of Ref. [17], we obtain the relevant polynomials as:

$$\left.\begin{array}{l}\tilde{\tau}(x)=1-z;\ \sigma(x)=x(1-x);\ \sigma^{/}(z)=1-2x,\ \sigma^{//}(x)=-2;\\ \sigma(x)=-(\varepsilon+\beta_3)x^2+(2\varepsilon+\beta_0-\beta_1+\beta_3)x-(\varepsilon-\beta_0-\beta_2+\gamma)\end{array}\right\} \tag{9}$$

Inserting the polynomials given by Eq. (9) into Eq. (11) of Ref. [17], gives the polynomial:

$$\pi(z)=-\frac{z}{2}\pm\sqrt{(\eta_1-K)z^2+(K+\eta_2)\mathrm{z}+\eta_3}, \tag{10}$$

where

$$\left.\eta_1=\left(\frac{1}{4}+\varepsilon+\beta_3\right),\ \eta_2=-(2\varepsilon-\beta_0-\beta_1+\beta_3),\ \eta_3=(\varepsilon-\beta_0-\beta_2+\gamma)\right\}. \tag{11}$$

According to the NU method, the quadratic form under the square root sign of Eq. (10) must be solved by setting the discriminant of this quadratic equation equal to zero: $\Delta=b^2-4ac=0$. This discriminant gives a new quadratic equation, which can be solved for the constant k to get the two roots. Here, we take the negative root given as:

$$K=-(\eta_2+2\eta_3)-2\sqrt{\eta_3}\sqrt{\eta_3+\eta_2+\eta_1}. \tag{12}$$

Substituting Eq. (12) into Eq. (10), $\pi(x)$ has the most suitable expression given as

$$\pi(x)=\frac{-x}{2}-\left[\left(\sqrt{\eta_3}+\sqrt{\eta_3+\eta_2+\eta_1}\right)x-\sqrt{\eta_3}\right], \tag{13}$$

using Eq. (9) and Eq. (13). Therefore, we obtain $\tau(x)$ and $\tau^{/}(x)$ as follows:

$$\tau(x)=1-2x-2\sqrt{\eta_3}x-2\sqrt{\eta_3+\eta_2+\eta_1}x+2\sqrt{\eta_3}, \tag{14}$$

$$\tau^{/}(x)=-2\left[1+\sqrt{\eta_3}+\sqrt{\eta_3+\eta_2+\eta_1}\right],\cdot \tag{15}$$

where $\tau^{/}(x)$ is the first derivative of $\tau(x)$. Referring to Eq. (10) and Eq. (13) of Ref. [17], the following expressions for λ_n and λ are as follows:

$$\lambda_n=n^2+\left[1+2\sqrt{\eta_3}+2\sqrt{\eta_3+\eta_2+\eta_1}\right]n,\ (n=0,1,2,...), \tag{16}$$

$$\lambda=-\frac{1}{2}-\sqrt{\eta_3}-\sqrt{\eta_3+\eta_2+\eta_1}-(\eta_2+2\eta_3)-2\sqrt{\eta_3}\sqrt{\eta_3+\eta_2+\eta_1}, \tag{17}$$

where n is the number of nodes in the radial wavefunctions ψ_{nl} .When comparing Eqs. (16) and (17) with the help of Eq. (8), we obtain bound state energy eigenvalues of Schrödinger equation with class of inversely quadratic plus Hulthén potential as:

$$E_{nl}=V_2\delta^2-V_0\delta-\frac{\delta^2\hbar^2 l(l+1)}{2\mu}-\frac{\delta^2\hbar^2}{8\mu}\left[\frac{\left(n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)+\frac{2\mu V_1}{\hbar^2}-\frac{2\mu V_2}{\hbar^2}}\right)^2-\frac{2\mu V_0}{\delta\hbar^2}-\frac{\mu V_2}{\hbar^2}-\frac{2\mu V_3}{\delta^2\hbar^2}+l(l+1)}{n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)+\frac{2\mu V_1}{\hbar^2}-\frac{2\mu V_2}{\hbar^2}}}\right]^2. \tag{18}$$

We can obtain the other part of the wave function $\phi(x)$ and weight function $\rho(x)$ by inserting the values of $\sigma(x)$, $\pi(x)$, and $\tau(x)$ given in Eqs. (9), (13) and (14), respectively, into Eq. (3) of foundations the theory of special functions and Eq.(3) of the basic properties of polynomials of hypergeometric type of Ref. [17] as follows:

$$\phi(x)=x^{\sqrt{\eta_3}}(1-x)^{\left(\frac{1}{2}+\sqrt{\eta_3+\eta_2+\eta_1}\right)}, \tag{19}$$

$$\rho(x)=x^{2\sqrt{\eta_3}}(1-x)^{2\sqrt{\eta_3+\eta_2+\eta_1}}. \tag{20}$$

By substituting Eqs. (9) and (20), into Eq. (2) of the basic properties of polynomials of hypergeometric type of Ref. [17], the Rodrigues relation is written as

$$y_n=B_n x^{-2\sqrt{\eta_3}}(1-x)^{-2\sqrt{\eta_3+\eta_2+\eta_1}}\frac{d^n}{dx^n}\left[x^{n+2\sqrt{\eta_3}}(1-x)^{n+2\sqrt{\eta_3+\eta_2+\eta_1}}\right], \tag{21}$$

where B_n is the Jacobi polynomial. Hence, the wave function becomes

$$\psi_{nl}(x)=\mathrm{N}_{nl}\,x^{\sqrt{\eta_3}}(1-x)^{\left(\frac{1}{2}+\sqrt{\eta_3+\eta_2+\eta_1}\right)}P_n^{\left(2\sqrt{\eta_3},2\sqrt{\eta_3+\eta_2+\eta_1}\right)}(1-2x), \tag{22}$$

where N_{nl} is the normalization constant. Using the normalization condition, we obtain the normalization constant as follows:

$$\frac{\mathrm{N}_{nl}^2}{\delta}\int_{-1}^{1}\left(\frac{1-y}{2}\right)^{2\sqrt{\eta_3}}\left(\frac{1+y}{2}\right)^{\varpi}\left[P_n^{\left(2\sqrt{\eta_3},2\varpi-1\right)}(y)\right]^2 dy=1, \tag{23}$$

where

$$\left.\begin{aligned}\varpi&=1+\sqrt{4\eta_3+4\eta_2+4\eta_1},\\ \varpi-1&=\sqrt{4\eta_3+4\eta_2+4\eta_1}\end{aligned}\right\}.$$

(24)

Comparing Eq. (25) with the standard integral of the form of Eq. (37) of [58],

$$\int_{-1}^{1}\left(\frac{1-p}{2}\right)^{u}\left(\frac{1+y}{2}\right)^{v}\left(P_n^{(2u,2v-1)}(p)\right)^2 dp=\frac{2\Gamma(u+n+1)\Gamma(v+n+1)}{n!u\Gamma(u+v+n+1)}. \tag{25}$$

Hence, we write the normalization constant as

$$\mathrm{N}_{nl}=\left[\frac{n!2\sqrt{\eta_3}\;\delta\,\Gamma\left(2\sqrt{\eta_3}+\sqrt{4\eta_3+4\eta_2+4\eta_1}+n+2\right)}{2\Gamma\left(2\sqrt{\eta_3}+n+1\right)\Gamma\left(\sqrt{4\eta_3+4\eta_2+4\eta_1}+n+2\right)}\right]^{\frac{1}{2}}. \tag{26}$$

Therefore, the complete eigenfunction can be express as:

$$\psi_{nl}(x)=\left[\frac{n!2\sqrt{\eta_3}\;\delta\,\Gamma\left(2\sqrt{\eta_3}+\sqrt{4\eta_3+4\eta_2+4\eta_1}+n+2\right)}{2\Gamma\left(2\sqrt{\eta_3}+n+1\right)\Gamma\left(\sqrt{4\eta_3+4\eta_2+4\eta_1}+n+2\right)}\right]^{\frac{1}{2}}x^{\sqrt{\eta_3}}(1-x)^{\left(\frac{1}{2}+\sqrt{\eta_3+\eta_2+\eta_1}\right)}P_n^{\left(2\sqrt{\eta_3},2\sqrt{\eta_3+\eta_2+\eta_1}\right)}(1-2x) \tag{27}$$

3. Discussion

In Table 1, we numerically reported the energy eigenvalues for the class of inversely quadratic plus Hulthén potential by varying the principal quantum number n at a fixed orbital angular momentum quantum number l with the potential strength ($V_0=1, \mathrm{V}_1=-1, V_2=-1, \mathrm{V}_3=0.025$ $V_0=2, \mathrm{V}_1=-3, V_2=-3, \mathrm{V}_3=0.05$) for $\delta=0.025$. For a fixed value of angular momentum quantum l, the energy spectrum increases as the principal quantum number n increases for this range of potential strength as the screening parameter is not varied. In Table 2, we numerically show the energy eigenvalues of this potential at a fixed n by varying l for various screening parameters, $\delta=0.05, 0.075,$ and 0.1. As the screening parameter and angular momentum quantum l increases for a fixed value of principal quantum number n, the energy spectrum increases. In Table 3, we numerically present energy eigenvalues of Hulthén potential at 2p, 3p, 3d, 4p. As the screening parameter increases, the energy eigenvalues increases with increase in the quantum numbers. We compared our result for the Hulthén potential with the results from three other methods.

In Tables 4, we numerically presented eigenvalues for four diatomic molecules using the energy equation given in Eq. (18). This was done by inputting the model parameters for each molecule presented in Table 4. These diatomic molecules were selected because of their important in chemistry and chemical physics. Furthermore, we have additionally utilized the accompanying transformations: $1\ \mathrm{amu}=931.494028\ \mathrm{MeV}/c^2$ and $\hbar c=1973.29\ \mathrm{eV}\,\overset{\circ}{\mathrm{A}}$ Oyewumi et al. [59]. The results show that the bound state energy spectra of these diatomic molecules increases as various quantum numbers n and l increases.

In Figs. 2 (a) and (b), we plotted the energy eigenvalues of a class of inversely quadratic plus Hulthén potential in the ground $n=0$ and the second excited $n=2$ states, respectively, for different $l,(l=0,1,2,3,4)$ as a function of Coulomb potential parameter. From the plot, the energy eigenvalue decreases, i.e., more attractive with an increase in orbital quantum number l. In Figs. 3 (a) and (b), we plotted energy eigenvalues of a class of inversely quadratic plus Hulthén potential as a function of inversely quadratic Yukawa potential strength V_1 in the ground $n=0$ and the second excited $n=2$ states, respectively, for various l. The plot shows that the energy eigenvalues increase as V_1 increase in both the ground and second excited states. In Figs. 4 (a) and (b), we graphically show the variation of the class of inversely quadratic plus Hulthén potential in the ground $n=0$ and the second excited $n=2$ states, respectively, for various l as a function of the potential strength of inversely quadratic potential V_2. We observed that the particle is more bounded in the ground state as the potential strength V_2 increases compared to the second excited state since the energy eigenvalues become less attractive in some states for $l=2,3$ and 4, respectively. In Figs. 5 (a) and (b), we plotted the energy spectra of the class of inversely quadratic plus Hulthén potential as a function of V_0 in the ground $n=0$ and the second excited $n=2$ states of N_2 molecule for various l. The plot shows that the energy eigenvalues decrease as V_0 increases in both the ground and second excited states showing that N_2 molecules are more attractive in the ground $n=0$ state compared to the second excited $n=2$ state. In Fig. 6 (a) and (b), we plotted energy spectra as a function of V_3 for various μ of the selected diatomic molecules in the ground and second excited states. Fig. 7(a) and (b) show a variation of energy spectra with V_3 for various δ of the selected diatomic molecules in the ground and second excited state. It is observed that the energy eigenvalues decrease as V_3 is increased various μ and δ.

Table 1 Bound states energy eigenvalues (eV) for the class of inversely quadratic plus Hulthén potential with $\hbar=2\mu=1, \delta=0.025$

n	l	$V_0=1, V_1=-1, V_2=-1, V_3=0.025$	$V_0=2, V_1=-2, V_2=-2, V_3=0.05$	$V_0=4, V_1=-4, V_2=-4, V_3=0.1$
0	0	-1.012851562	-4.000625000	-15.90140625
1	0	-0.2726660156	-1.038476562	-4.051406250
2	0	-0.1362890625	-0.4906250000	-1.857656250
3	0	-0.08937744140	-0.2996972656	-1.090664062
4	0	-0.06856406250	-0.2122250000	-0.7365562500
0	1	-0.2622753906	-1.015664062	-4.003750000
1	1	-0.1327126736	-0.4815277778	-1.837517361
2	1	-0.08818603515	-0.2954003906	-1.080156250
3	1	-0.06847656250	-0.2101500000	-0.7305062500
4	1	-0.05872504340	-0.1647960070	-0.5415277778
0	2	-0.1259765625	-0.4637500000	-1.797656250
1	2	-0.08603759765	-0.2870410156	-1.059375000
2	2	-0.06845156250	-0.2061500000	-0.7185562500
3	2	-0.05985351562	-0.1631640625	-0.5343750000
4	2	-0.05566406250	-0.1382397959	-0.4243144132
0	3	-0.08340087890	-0.2750878906	-1.028789062
1	3	-0.06878906250	-0.2005250000	-0.7010062500
2	3	-0.06180664062	-0.1609765625	-0.5239062500
3	3	-0.05859135842	-0.1381250000	-0.4181154336
4	3	-0.05752990723	-0.1243188476	-0.3504785156
0	4	-0.06993906250	-0.1937250000	-0.6783062500
1	4	-0.06489691840	-0.1585460070	-0.5104340278
2	4	-0.06285156250	-0.1383290816	-0.4102072704
3	4	-0.06254943848	-0.1262329102	-0.3461816406
4	4	-0.06339168596	-0.1189891975	-0.3033352624

Table 2 Bound states energy eigenvalues (eV) for the of class of inversely quadratic plus Hulthén potential with $\hbar=\mu=1$ $V_0=2, V_1=-3, V_2=-3, V_3=0.05$

n	l	$\delta=0.05$	$\delta=0.075$	$\delta=0.1$
0	0	−4.455000000	−3.541805556	−3.145000000
0	1	−1.215078125	−1.058752170	−1.035312500
0	2	−0.6187500000	−0.6122492285	−0.6722222222
0	3	−0.4197070312	−0.4794536676	−0.5882031250
0	4	−0.3398000000	−0.4462722222	−0.6002000000
1	0	−1.247578125	−1.097502170	−1.077812500
1	1	−0.6426388889	−0.6354436729	−0.6900000000
1	2	−0.4337695312	−0.4853130426	−0.5788281250
1	3	−0.3450000000	−0.4359722222	−0.5650000000
1	4	−0.3073003472	−0.4341148245	−0.6028125000
2	0	−0.6550000000	−0.6479783951	−0.7005555555
2	1	−0.4439257812	−0.4909771051	−0.5757031250
2	2	−0.3499500000	−0.4306097222	−0.5428000000
2	3	−0.3063281250	−0.4166495467	−0.5600347222
2	4	−0.2896938776	−0.4312613379	−0.6123469388
3	0	−0.4492382812	−0.4943364801	−0.5750781250
3	1	−0.3537500000	−0.4281597222	−0.5300000000
3	2	−0.3063281250	−0.4051912134	−0.5308680556
3	3	−0.2850000000	−0.4094756236	−0.5650000000
3	4	−0.2803173828	−0.4340235731	−0.6267382812
4	0	−0.3558000000	−0.4272722222	−0.5242000000
4	1	−0.3066753472	−0.3983335745	−0.5128125000
4	2	−0.2820153061	−0.3943416950	−0.5316326531
4	3	−0.2732080078	−0.4094337294	−0.5764257812
4	4	−0.2759876543	−0.4406395748	−0.6450000000

Table 3 Bound states energy eigenvalues (eV) of the Hulthén potential as a function of the screening Parameters δ for 2p, 3p, 3d, and 4p states and for $Z=1$ in atomic units $(\hbar=\mu=e=1)$.

State	δ	Present (NU)	AIM [60]	EQR [61]	SUSY [62]
2p	0.025	−0.1128125000	-0.1128125	-0.1128125	-0.1127605
	0.050	−0.1012500000	-0.1012500	-0.1012500	-0.1010425
	0.075	−0.09031249994	-0.0903125	-0.0903125	-0.0898478
	0.10	−0.08000000000	-0.0800000	-0.0800000	-0.0791794
	0.15	−0.06124999998	-0.0612500	-0.0612500	-0.0594415
3p	0.025	−0.04070312500	-0.0437590	-0.0437590	-0.0437068
	0.050	-0.03336810000	-0.0333681	-0.0333681	-0.0331632
	0.075	-0.02438370000	-0.0243837	-0.0243837	-0.0239331
	0.10	-0.01680560000	-0.0168056	-0.0168056	-0.0160326
	0.15	-0.00586810000	-0.0058681	-0.0058681	-0.0043599
3d	0.025	-0.04360440000	-0.0437587	-0.0437587	-0.0436030
	0.050	-0.03275080000	-0.0333681	-0.0333681	-0.0327532
	0.075	-0.02299480000	-0.0243837	-0.0243837	-0.0230306
	0.10	-0.01433640000	-0.0162600	-0.0162600	-0.0144832
	0.15	-0.00031240000	-0.0058681	-0.0058681	-0.0132820
4p	0.025	-0.01994860000	-0.0200000	-0.0200000	-0.0199480
	0.050	-0.01104420000	-0.0112500	-0.0112500	-0.0110430
	0.075	-0.00453700000	-0.0050000	-0.0050000	-0.0045385
	0.10	-0.00042690000	-0.0012500	-0.0012500	-0.0004434

Table 4 Spectroscopic parameters of the molecules used in this work [59]

Molecule	$\alpha\left(\overset{0}{\mathrm{A}}\right)^{-1}$	$\mu(\mathrm{amu})$	$\mu(\mathrm{eV})$
N_2	2.69860	7.0033500000	0.6523578701
O_2	1.295515	7.9974575040	0.74495839042
NO	2.75340	7.4684410000	0.69568081900
CO	2.29940	6.8605860000	0.63905948876

Table 5 Energy spectra (in eV) of class of inversely quadratic plus Hulthen potential for $V_0=1,\ V_1=V_2=-1, V_3=0.025$ and $\hbar c=1973.29 eV\,\overset{0}{\mathrm{A}}$ for N_2, O_2, NO and CO diatomic molecules

n	l	N_2	O_2	NO	CO
0	0	−102.7119268	−23.19497264	−126.7384336	−20.57424584
0	1	−30.30849598	−9.453142109	−36.45622154	−8.798919265
0	2	−16.95021661	−6.930212578	−19.79018435	−6.641819365
0	3	−12.30628452	−6.063890161	−13.98924338	−5.905643942
0	4	−10.18475382	−5.679164767	−11.33218294	−5.583549884
0	5	−9.059727937	−5.486789797	−9.915958908	−5.427786332
1	0	−30.07202715	−9.368846178	−36.19627464	−8.713879144
1	1	−16.73132841	−6.849755612	−19.55063368	−6.559784975
1	2	−12.11100219	−5.989268264	−13.77677931	−5.828574813
1	3	−10.00628951	−5.607970361	−11.13933831	−5.509021515
1	4	−8.892132746	−5.416928527	−9.736182578	−5.353695279
1	5	−8.247963204	−5.317833657	−8.917746069	−5.278508861
2	0	−16.62260878	−6.809987732	−36.19627464	−6.519304712
2	1	−11.98217237	−5.940383964	−19.55063368	−5.778202139
2	2	−9.874266958	−5.555735276	−13.77677931	−5.454478305
2	3	−8.760230009	−5.362421323	−11.13933831	−5.296033229
2	4	−8.116182734	−5.261007963	−9.736182578	−5.217664321
2	5	−7.724662434	−5.210441659	−8.917746069	−5.184264747
3	0	−11.91816497	−5.916200905	−13.56670214	−5.753317826
3	1	−9.787121287	−5.521464611	−10.90210156	−5.418760482
3	2	−8.662570784	−5.322346977	−9.489446311	−5.253726320
3	3	−8.012355153	−5.216562617	−8.666361658	−5.170172128
3	4	−7.616127092	−5.162076555	−8.158300703	−5.132017704
3	5	−7.369538341	−5.139134138	−7.835113863	−5.122355833
4	0	−9.743809264	−5.504495097	−10.85516342	−5.401094865
4	1	−8.598068359	−5.296014583	−9.420011074	−5.225969157
4	2	−7.935415930	−5.183820812	−8.584125641	−5.135243324
4	3	−7.530521367	−5.124161742	−8.067455968	−5.091126140
4	4	−7.276939786	−5.096569587	−7.737532584	−5.076003205
4	5	−7.119236710	−5.090491185	−7.525275330	−5.080827207

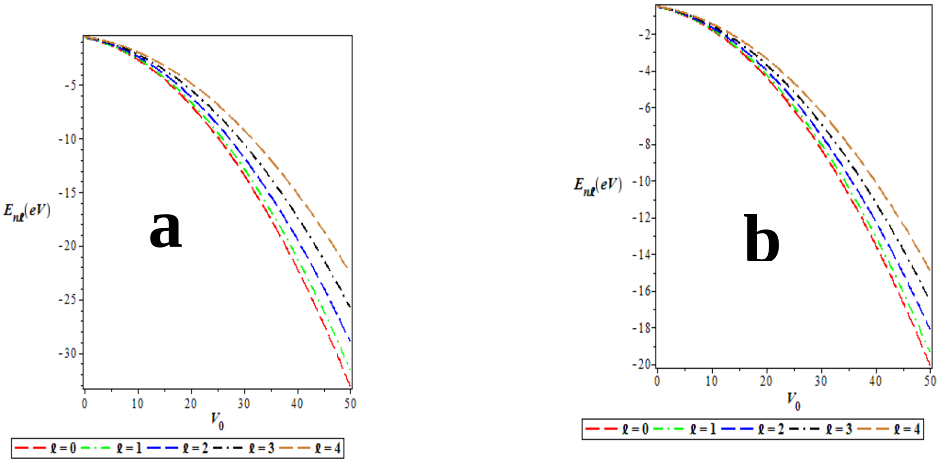

Fig. 2 (a) Variation of the ground state energy spectra for various l as a function of V_0. (b) The plot of the second excited state energy spectra for different l as a function of V_0. We choose $V_0 = 2,\ V_1 = -1,\ V_2 = -20,\ V_3 = 0.10$ and $\delta = 0.025$ for the ground and second excited states

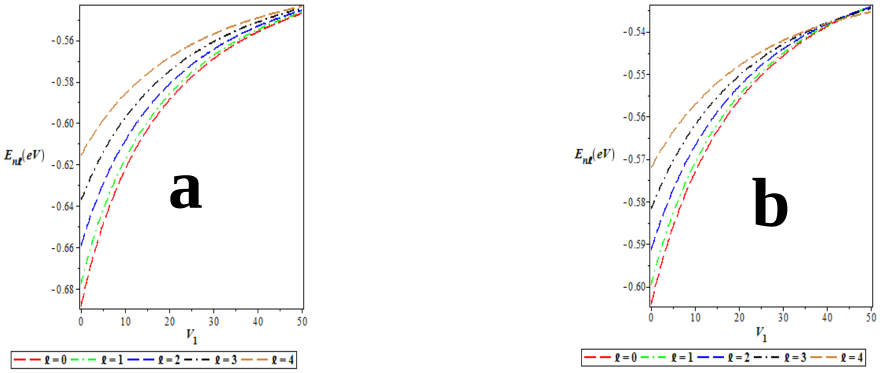

Fig. 3 (a) Variation of the ground state energy spectra for various l as a function of V_1. (b) The plot of the second excited state energy spectra for different l as a function of V_1. We choose $V_0 = 2,\ V_1 = -1,\ V_2 = -1,\ V_3 = 0.10$ and $\delta = 0.025$ for the ground and second excited states.

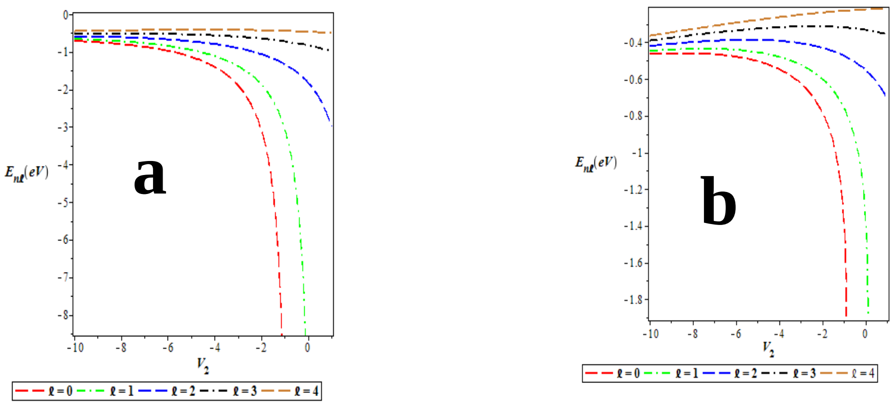

Fig. 4 (a) Variation of the ground state energy spectra for various l as a function V_2. (b). The plot of the second excited state energy spectra for different l as a function of V_2. We choose $V_0 = 2,\ V_1 = -1,\ V_2 = -2,\ V_3 = 0.10$ and $\delta = 0.025$ for the ground and second excited states.

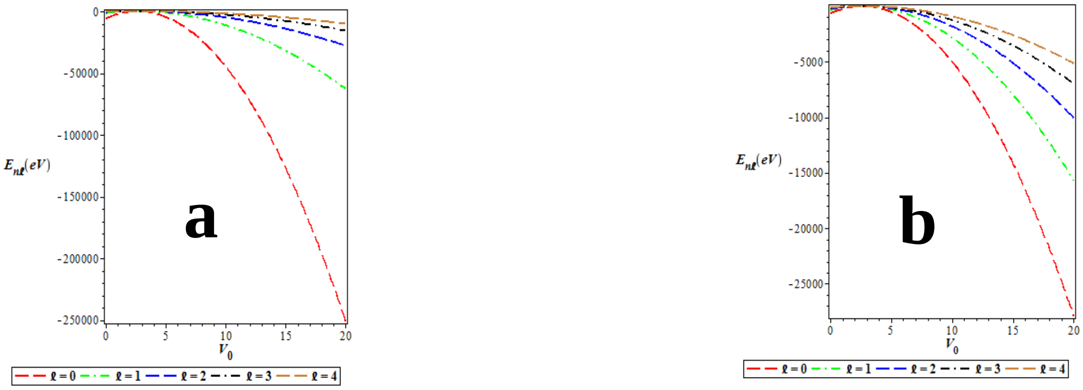

Fig. 5 (a) Variation of the ground state energy spectra of N_2 for various l as a function of V_0. (b) The plot of the second excited state energy spectra of N_2 for different l as a function of V_0. We choose $V_0 = 2,\ V_1 = -1,\ V_2 = -2,\ V_3 = 0.10$ and $\delta = 0.025$ for the ground and second excited states

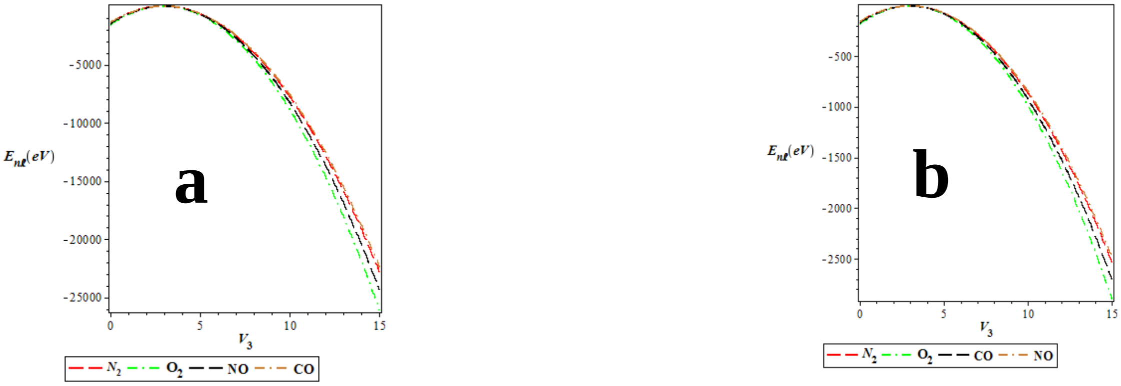

Fig. 6 (a) Energy eigenvalues variation with V_3 for various μ of the selected diatomic molecules in the ground state (b) The plot of the second excited state energy spectra for various μ of the selected diatomic molecules a function of V_3.

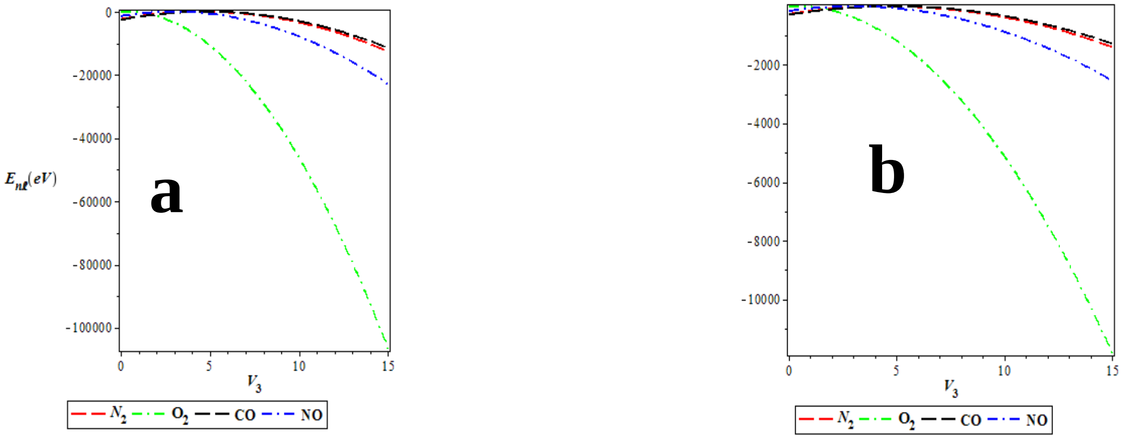

Fig. 7(a) Energy eigenvalues variation with V_3 for various δ of the selected diatomic molecules in the ground state (b) The plot of the second excited state energy spectra for various δ of the selected diatomic molecules a function of V_3.

Special cases

1. When we set $V_0 = V_1 = V_2 = 0$ in Eq. (21), we obtain the energy eigenvalues for the Hulthén potential,

$$E_{nl}=-\frac{\delta^2\hbar^2 l(l+1)}{2\mu}-\frac{\alpha^2\hbar^2}{8\mu}\left[\frac{(n+l+1)^2+l(l+1)-\frac{2\mu V_3}{\delta^2\hbar^2}}{(n+l+1)}\right]^2. \tag{28}$$

Equation (40) is in agreement with Eq. (32) of [63]; Eq. (24) of [64]; Eq. (28) of [65]; Eq. (37) of [66] and Eq. (20) of [44].

2. If we set $V_0=V_1=V_3=0$ in Eq. (21), we obtain the energy eigenvalues for the inversely quadratic potential,

$$E_{nl}=V_2\delta^2-\frac{\delta^2\hbar^2 l(l+1)}{2\mu}-\frac{\alpha^2\hbar^2}{8\mu}\left[\frac{\left(n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)-\frac{2\mu V_2}{\hbar^2}}\right)^2-\frac{4\mu V_2}{\hbar^2}+l(l+1)}{n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)-\frac{2\mu V_2}{\hbar^2}}}\right]^2. \tag{29}$$

3. If we set $V_0=V_2=V_3=0$ in Eq. (21), we obtain the energy eigenvalues for the inversely quadratic Yukawa potential,

$$E_{nl}=-\frac{\delta^2\hbar^2 l(l+1)}{2\mu}-\frac{\alpha^2\hbar^2}{8\mu}\left[\frac{\left(n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)+\frac{2\mu V_1}{\hbar^2}}\right)^2+\frac{2\mu V_1}{\hbar^2}+l(l+1)}{n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)+\frac{2\mu V_1}{\hbar^2}}}\right]^2. \tag{30}$$

Equation (30) agrees with Eq. (33) of [44].

4. If we set $V_0=V_1=V_2=V_3=\delta=0$ in Eq. (21), we obtain the energy eigenvalues for Coulomb potential,

$$E_{np}=\frac{Z^2e^4\mu}{2\hbar^2(n+l+1)^2}. \tag{31}$$

Where $V_0=Ze^2$ is the nuclear charge. Equation (31) agrees with Eq. (39) of [18]; Eq. (16) of [67] and Eq. (24) of [68].

5. If we set $V_2=V_3=0$ in Eq. (21), we obtain the energy eigenvalues for inversely quadratic Hellmann potential,

$$E_{nl}=-V_0\delta-\frac{\delta^2\hbar^2 l(l+1)}{2\mu}-\frac{\alpha^2\hbar^2}{8\mu}\left[\frac{\left(n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)+\frac{2\mu V_1}{\hbar^2}}\right)^2-\frac{2\mu V_0}{\alpha\hbar^2}+\frac{2\mu V_1}{\hbar^2}+l(l+1)}{n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)+\frac{2\mu V_1}{\hbar^2}}}\right]^2. \tag{32}$$

Equation (30) agrees with Eq. (34) of [44] and Eq. (29) of [68].

6. If we set $V_2=0$ in Eq. (21), we obtain the energy eigenvalues for inversely quadratic Hellmann plus inversely quadratic Yukawa potential,

$$E_{nl}=-V_0\delta-\frac{\delta^2\hbar^2 l(l+1)}{2\mu}-\frac{\alpha^2\hbar^2}{8\mu}\left[\frac{\left(n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)+\frac{2\mu V_1}{\hbar^2}}\right)^2-\frac{2\mu V_0}{\alpha\hbar^2}+\frac{2\mu V_1}{\hbar^2}+l(l+1)}{n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)+\frac{2\mu V_1}{\hbar^2}}}\right]^2. \tag{33}$$

Equation (33) agrees with Eq. (29) of [44] and Eq. (22) of [68].

7. If we set $V_3=0$ in Eq. (21), we obtain the energy eigenvalues for inversely quadratic Hellmann potential plus inversely quadratic potential,

$$E_{nl}=V_2\delta^2-V_0\delta-\frac{\delta^2\hbar^2 l(l+1)}{2\mu}-\frac{\alpha^2\hbar^2}{8\mu}\left[\frac{\left(n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)+\frac{2\mu V_1}{\hbar^2}-\frac{2\mu V_2}{\hbar^2}}\right)^2-\frac{2\mu V_0}{\alpha\hbar^2}+\frac{2\mu V_1}{\hbar^2}-\frac{4\mu V_2}{\hbar^2}+l(l+1)}{n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)+\frac{2\mu V_1}{\hbar^2}-\frac{2\mu V_2}{\hbar^2}}}\right]^2. \tag{34}$$

8. If we set $V_0=V_1=0$ in Eq. (21), we obtain the energy eigenvalues for inversely quadratic potential plus inversely quadratic Yukawa potential,

$$E_{nl}=V_2\delta^2-\frac{\delta^2\hbar^2 l(l+1)}{2\mu}-\frac{\alpha^2\hbar^2}{8\mu}\left[\frac{\left(n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)-\frac{2\mu V_2}{\hbar^2}}\right)^2-\frac{4\mu V_2}{\hbar^2}+l(l+1)}{n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)-\frac{2\mu V_2}{\hbar^2}}}\right]^2. \tag{35}$$

Conclusion

The bound state solutions to the Schrödinger equation with the newly proposed potential of a class of inversely quadratic plus Hulthén potential have been studied within the Greene-Aldrich approximation scheme. The eigenvalues and the normalized eigenfunctions are obtained using the NU method. We then apply the solution for four diatomic molecules by imputing the experimental values of each molecular parameter. The results show that the bound state energy spectra of these diatomic molecules increases as various quantum numbers n and l increase. There is a variation of the ground state energies compared to those of the second excited states (see **Figs. 2– 7**).

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