East European Journal of Physics. 3. 158-166 (2023)
DOI:10.26565/2312-4334-2023-3-12 ISSN 2312-4334

BOUND STATE AND RO-VIBRATIONAL ENERGIES EIGENVALUES OF SELECTED DIATOMIC MOLECULES WITH A CLASS OF INVERSELY QUADRATIC YUKAWA PLUS HULTHÉN POTENTIAL MODEL†

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Received July 7, 2023; revised July 17, 2023; accepted July 18, 2023

The Nikiforov-Uvarov approach is used in this study to solve the Schrödinger equation utilizing a class of inversely quadratic Yukawa plus Hulthén potential model with an approximation to the centrifugal term. The normalized wave function and energy eigenvalue equation were obtained. The numerical bound state for a few diatomic molecules (N_2, O_2, NO, and CO) for various rotational and vibrational quantum numbers was calculated using the energy equation and the related spectroscopic data. Our results show that, with no divergence between the s-wave and l-wave, the energy eigenvalues are very sensitive to the potential and diatomic molecule properties, suggesting that the approximation approach is appropriate for this set of potentials. The results are consistent with earlier studies in the literature, and we also found four special cases of this potential.
Keywords: *Schrödinger equation; Nikiforov-Uvarov method; Class of inversely quadratic plus Hulthén potential; Diatomic molecules; Bound state*
PACS: 31.15.-p

INTRODUCTION

The time-independent Schrödinger wave equation can be used to study the dynamics and interactions of quantum mechanical processes and non-relativistic spinless particles [1-4]. Because the eigenvalues and eigenfunctions associated with quantum problems include essential information regarding the quantum system. The analytical solutions to this equation with physical potentials are likely to play an important role in our understanding of the underlying principles of a quantum system [5, 6]. The bound state solutions of the Schrödinger equation for a few of these potentials, such as the Coulomb potential (CP) [7], Woods-Saxon [8], Hulthén [9], Manning-Rosen [10], and so on, are possible in some situations. A suitable approximation scheme can also be used to solve the Schrödinger equation approximately when the arbitrary rotational momentum quantum number is available [11]. 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 the improved approximation scheme in Ref. [16] are a few examples of these approximations.

To find the exact and approximate solutions to the Schrödinger equation, quantum mechanical techniques have been extensively used over time by scholars [17–27]. Inversely quadratic Hellmann potential (IQHP) has been used by numerous authors in different areas of physics [28-31]. Another intriguing potential is inversely quadratic potential (IQP). The inversely quadratic potential has been used by Oyewumi and Bangudu [32] and several authors in the literature [33-35].

In order to investigate the interaction that exists between two particles, the Hulthén potential (HP) [36] is essential. It is utilized in the study of atomic, condensed matter, nuclear, and molecular physics as well as chemical physics [37,38]. Another potential of interest is a newly proposed potential by Inyang et al. [39] called the class of inversely quadratic Yukawa potential. This work aims to use the class of inversely quadratic Yukawa plus Hulthén potential (CIQYHP) to obtain bound state approximate solutions to the Schrödinger equation. The obtain energy equation will be used to investigate the ro-vibrational energies of some selected diatomic molecules and the bound state energies. The potential model under study is of the form:

$$V(r) = -\frac{V_{01}}{r} + \frac{V_{21}e^{-\delta_0 r}}{r^2} - \frac{V_{11}}{r^2} - \frac{V_{31}e^{-\delta_0 r}}{1-e^{-\delta_0 r}}, \tag{1}$$

where V_{01}, V_{11}, V_{21}, and V_{31} are potential strength and δ_0 is the screening parameter.

The shape of this potential as a function of the screening parameter is given in Fig. 1. The following is how the paper is set up: The energy eigenvalues and normalized eigenfunctions are obtained by solving the Schrödinger equation with the class of inversely quadratic Yukawa plus Hulthén potential using the Nikiforov-Uvarov method in Section 2. The resulting energy equation will be applied in Section 3 to compute numerically the energy eigenvalues at various states of the chosen diatomic molecules and the discussion. In Section 4, conclusions are provided.

† ***Cite as:*** Fina O. Faithpraise, Etido P. Inyang, East Eur. J. Phys. 3, 158 (2023), https://doi.org/10.26565/2312-4334-2023-3-12

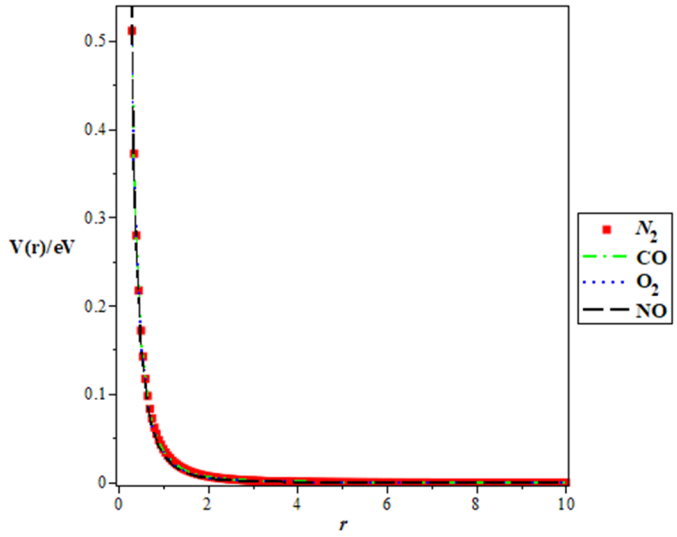

Figure 1. Variation of the potential $V(r)$ against internuclear distance r for the N_2, O_2, NO and CO diatomic molecules

2. APPROXIMATE SOLUTION OF SCHRÖDINGER EQUATION WITH THE CLASS OF INVERSELY QUADRATIC YUKAWA PLUS HULTHÉN POTENTIAL

In this study, the second-order differential equation of the hypergeometric type is solved using the Nikiforov-Uvarov method. The specifics are provided in Reference [17]. The Schrödinger equation reads [40]

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

where $\psi_{nl}(r)$ is the wavefunctions, E_{nl} is the eigenvalues of the quantum system, r is the radial distance from the origin, $\hbar$ is the reduced Planck's constant and μ is the reduced mass. Replacing Eq. (1) into Eq. (2) gives

$$\frac{d^2\psi_{nl}(r)}{dr^2} + \left[\frac{2\mu E_{nl}}{\hbar^2} + \frac{2\mu V_{01}}{\hbar^2 r} - \frac{2\mu V_{11}e^{-\delta_0 r}}{\hbar^2 r^2} + \frac{2\mu V_{21}}{\hbar^2 r^2} + \frac{2\mu V_{31}e^{-\delta_0 r}}{\hbar^2\left(1-e^{-\delta_0 r}\right)} - \frac{l(l+1)}{r^2}\right]\psi_{nl}(r) = 0 \tag{3}$$

Equation (3) cannot be solved with the proposed potential because of the inverse square term. We then introduce the Greene-Aldrich approximation scheme [11] to deal with the inverse square term. This approximation scheme is a good approximation and is valid for $\delta_0 << 1$, and it becomes

$$\frac{1}{r^2} \approx \frac{{\delta_0}^2}{\left(1-e^{-\delta_0 r}\right)^2}. \tag{4}$$

Applying Eq. (5), we have

$$\frac{d^2\psi_{nl}(r)}{dr^2} + \left[\frac{2\mu E_{nl}}{\hbar^2} + \frac{2\mu V_{01}\delta_0}{\hbar^2\left(1-e^{-\delta_0 r}\right)} - \frac{2\mu V_{11}{\delta_0}^2 e^{-\delta_0 r}}{\hbar^2\left(1-e^{-\delta_0 r}\right)^2} + \frac{2\mu V_{21}{\delta_0}^2}{\hbar^2\left(1-e^{-\delta_0 r}\right)^2} + \frac{2\mu V_{31}e^{-\delta_0 r}}{\hbar^2\left(1-e^{-\delta_0 r}\right)} - \frac{{\delta_0}^2 l(l+1)}{\left(1-e^{-\delta_0 r}\right)^2}\right]\psi_n(r) = 0\,. \tag{5}$$

By using the change of variable from $r \to x_b$, new coordinate is

$$x_b = e^{-\delta_0 r}. \tag{6}$$

We put Eq. (6) into Eq. (5) and simplify to get,

$$\frac{d^2\psi(x_b)}{{dx_b}^2} + \frac{1-x_b}{x_b(1-x_b)}\frac{d\psi(x_b)}{dx_b} + \frac{1}{\left[x_b(1-x_b)\right]^2}\left[\begin{matrix}-(\varepsilon+\beta_{30}){x_b}^2 + (2\varepsilon+\beta_{00}-\beta_{10}+\beta_{30})x_b \\ -(\varepsilon-\beta_{00}-\beta_{20}+\gamma)\end{matrix}\right]\psi(x_b) = 0, \tag{7}$$

where

$$-\varepsilon=\frac{2\mu E_{nl}}{\delta_0{}^2\hbar^2},\quad \beta_{00}=\frac{2\mu V_{01}}{\delta_0\hbar^2},\quad \beta_{10}=\frac{2\mu V_{11}}{\hbar^2},\quad \beta_{20}=\frac{2\mu V_{21}}{\hbar^2},\quad \beta_{30}=\frac{2\mu V_{31}}{\delta_0{}^2\hbar^2},\quad \gamma=l(l+1)\Big\}. \tag{8}$$

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

$$\left.\begin{aligned}&\tilde{\tau}(x_b)=1-x_b;\ \sigma(x_b)=x_b(1-x_b);\ \sigma^{/}(x_b)=1-2x_b,\ \sigma^{//}(x_b)=-2;\\&\tilde{\sigma}(x_b)=-(\varepsilon+\beta_{30})x_b{}^2+(2\varepsilon+\beta_{00}-\beta_{10}+\beta_{30})x_b-(\varepsilon-\beta_{00}-\beta_{20}+\gamma)\end{aligned}\right\} \tag{9}$$

Inserting Eq. (9) into Eq. (11) of Ref. [17], gives;

$$\pi(x_b)=-\frac{x_b}{2}\pm\sqrt{(\eta_{01}-K_0)x_b{}^2+(K_0+\eta_{02})x_b+\eta_{03}}, \tag{10}$$

where

$$\eta_{01}=\left(\frac{1}{4}+\varepsilon+\beta_{30}\right),\ \eta_{02}=-(2\varepsilon-\beta_{00}-\beta_{10}+\beta_{30}),\ \eta_{03}=(\varepsilon-\beta_{00}-\beta_{20}+\gamma)\Big\}. \tag{11}$$

The NU approach states that the discriminant of this quadratic equation must be set to zero in order to solve the quadratic form of Eq. (10) under the square root sign. A new quadratic equation is generated by this discriminant, which can be solved for the constant K_0 to obtain the two roots:

$$K_0=-(\eta_{02}+2\eta_{03})-2\sqrt{\eta_{03}}\sqrt{\eta_{03}+\eta_{02}+\eta_{01}}. \tag{12}$$

Replacing Eq. (12) into Eq. (10), $\pi(x_b)$ has the expression given as

$$\pi(x_b)=-\frac{x_b}{2}-\left[\left(\sqrt{\eta_{03}}+\sqrt{\eta_{03}+\eta_{02}+\eta_{01}}\right)x_b-\sqrt{\eta_{03}}\right], \tag{13}$$

with Eq. (9) and Eq. (13). Therefore, we obtain

$$\tau(x_b)=1-2x_b-2\sqrt{\eta_{03}}x_b-2\sqrt{\eta_{03}+\eta_{02}+\eta_{01}}x_b+2\sqrt{\eta_{03}}, \tag{14}$$

$$\tau^{/}(x_b)=-2\left[1+\sqrt{\eta_{03}}+\sqrt{\eta_{03}+\eta_{02}+\eta_{01}}\right], \tag{15}$$

Referring to Eq. (10) and Eq. (13) of Ref. [17], we have the following equations:

$$\lambda_n=n^2+\left[1+2\sqrt{\eta_{03}}+2\sqrt{\eta_{03}+\eta_{02}+\eta_{01}}\right]n, \tag{16}$$

$$\lambda=-\frac{1}{2}-\sqrt{\eta_{03}}-\sqrt{\eta_{03}+\eta_{02}+\eta_{01}}-(\eta_{02}+2\eta_{03})-2\sqrt{\eta_{03}}\sqrt{\eta_{03}+\eta_{02}+\eta_{01}}, \tag{17}$$

With the aid of Eq. (8), we can compare Eqs. (16) and (17) and get the bound state energy eigenvalues of the Schrödinger equation with the class of inversely quadratic Yukawa plus Hulthén potential as follows:

$$E_{nl}=V_{21}\delta_0{}^2-V_{01}\delta_0-\frac{\delta_0{}^2\hbar^2 l(l+1)}{2\mu}-\frac{\delta_0{}^2\hbar^2}{8\mu}\left[\frac{\left(n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)+\frac{2\mu V_{11}}{\hbar^2}-\frac{2\mu V_{21}}{\hbar^2}}\right)^2-\frac{2\mu V_{01}}{\delta_0\hbar^2}-\frac{\mu V_{21}}{\hbar^2}-\frac{2\mu V_{31}}{\delta_0{}^2\hbar^2}+l(l+1)}{n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)+\frac{2\mu V_{11}}{\hbar^2}-\frac{2\mu V_{21}}{\hbar^2}}}\right]^2. \tag{18}$$

Therefore, the complete eigenfunction can be express as:

$$\psi_{nl}(x_b)=\left[\frac{n!2\sqrt{\eta_{03}}\ \delta_0\ \Gamma\left(2\sqrt{\eta_{03}}+\sqrt{4\eta_{03}+4\eta_{02}+4\eta_{01}}+n+2\right)}{2\Gamma\left(2\sqrt{\eta_{03}}+n+1\right)\Gamma\left(\sqrt{4\eta_{03}+4\eta_{02}+4\eta_{01}}+n+2\right)}\right]^{\frac{1}{2}} \tag{19}$$
$$x_b^{\sqrt{\eta_{03}}}\left(1-x_b\right)^{\left(\frac{1}{2}+\sqrt{\eta_{03}+\eta_{02}+\eta_{01}}\right)}P_n^{\left(2\sqrt{\eta_{03}},2\sqrt{\eta_{03}+\eta_{02}+\eta_{01}}\right)}\left(1-2x_b\right)$$

Special cases

1. Setting $V_{01}=V_{11}=V_{21}=0$ in Eq. (18), we obtain the energy equation for the Hulthén potential,

$$E_{nl}=-\frac{\delta_0^{\,2}\hbar^2 l(l+1)}{2\mu}-\frac{\delta_0^{\,2}\hbar^2}{8\mu}\left[\frac{(n+l+1)^2+l(l+1)-\frac{2\mu V_{31}}{\delta_0^{\,2}\hbar^2}}{(n+l+1)}\right]^2. \tag{20}$$

Equation (20) is in agreement with Eq. (32) of [41] and Eq. (37) of [42].

2. Setting $V_{01}=V_{11}=V_{31}=0$ in Eq. (18), we obtain the energy equation for the inversely quadratic potential

$$E_{nl}=V_{21}\delta_0^{\,2}-\frac{\delta_0^{\,2}\hbar^2 l(l+1)}{2\mu}-\frac{\delta_0^{\,2}\hbar^2}{8\mu}\left[\frac{\left(n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)-\frac{2\mu V_{21}}{\hbar^2}}\right)^2-\frac{4\mu V_{21}}{\hbar^2}+l(l+1)}{n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)-\frac{2\mu V_{21}}{\hbar^2}}}\right]^2. \tag{21}$$

3. Setting $V_{01}=V_{11}=V_{21}=V_{31}=\delta_0=0$ in Eq. (18), we obtain the energy equation for Coulomb potential,

$$E_{nl}=\frac{Z^2e^4\mu}{2\hbar^2(n+l+1)^2}, \tag{22}$$

where $V_{01}=Ze^2$ is the nuclear charge. Equation (22) agrees with Eq. (24) of [46].

4. Setting $V_{21}=V_{31}=0$ in Eq. (18), we obtain the energy equation for IQHP,

$$E_{nl}=-V_{01}\delta_0-\frac{\delta_0^{\,2}\hbar^2 l(l+1)}{2\mu}-\frac{\delta_0^{\,2}\hbar^2}{8\mu}\left[\frac{\left(n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)+\frac{2\mu V_{11}}{\hbar^2}}\right)^2-\frac{2\mu V_{01}}{\delta_0\hbar^2}+\frac{2\mu V_{11}}{\hbar^2}+l(l+1)}{n+\frac{1}{2}+\sqrt{\frac{1}{4}+l(l+1)+\frac{2\mu V_{11}}{\hbar^2}}}\right]^2. \tag{23}$$

Equation (23) agrees with Eq. (29) of [46].

3. Results and Discussion

We numerically computed the energy eigenvalues for the class of inversely quadratic Yukawa plus Hulthén potential in Table 1 through adjusting the principal quantum number at a fixed orbital angular momentum quantum number with the potential strength ($V_{01}=1, V_{11}=-1, V_{21}=-1, V_{31}=0.025, V_{01}=2, V_{11}=-3, V_{21}=-3, V_{31}=0.05$) for $\delta_0=0.025$. 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.

Table 1. Energy bound states (eV) for the class of inversely quadratic Yukawa plus Hulthén potential with $\hbar=2\mu=1$, $\delta_0=0.025$

n	l	$V_{01}=1, V_{11}=-1,$ $V_{21}=-1, V_{31}=0.025$	$V_{01}=2, V_{11}=-2,$ $V_{21}=-2, V_{31}=0.05$	$V_{01}=4, V_{11}=-4,$ $V_{21}=-4, V_{31}=0.1$
0	0	-1.012851562	-4.000625000	-15.90140625
1		-0.2726660156	-1.038476562	-4.051406250
2		-0.1362890625	-0.4906250000	-1.857656250
3		-0.08937744140	-0.2996972656	-1.090664062
4		-0.06856406250	-0.2122250000	-0.7365562500

n	l	$V_{01}=1, V_{11}=-1,$ $V_{21}=-1, V_{31}=0.025$	$V_{01}=2, V_{11}=-2,$ $V_{21}=-2, V_{31}=0.05$	$V_{01}=4, V_{11}=-4,$ $V_{21}=-4, V_{31}=0.1$
0	1	-0.2622753906	-1.015664062	-4.003750000
1		-0.1327126736	-0.4815277778	-1.837517361
2		-0.08818603515	-0.2954003906	-1.080156250
3		-0.06847656250	-0.2101500000	-0.7305062500
4		-0.05872504340	-0.1647960070	-0.5415277778
0	2	-0.1259765625	-0.4637500000	-1.797656250
1		-0.08603759765	-0.2870410156	-1.059375000
2		-0.06845156250	-0.206150000	-0.7185562500
3		-0.05985351562	-0.1631640625	-0.5343750000
4		-0.05566406250	-0.1382397959	-0.4243144132
0	3	-0.08340087890	-0.2750878906	-1.028789062
1		-0.06878906250	-0.2005250000	-0.7010062500
2		-0.06180664062	-0.1609765625	-0.5239062500
3		-0.05859135842	-0.1381250000	-0.4181154336
4		-0.05752990723	-0.1243188476	-0.3504785156
0	4	-0.06993906250	-0.1937250000	-0.6783062500
1		-0.06489691840	-0.1585460070	-0.5104340278
2		-0.06285156250	-0.1383290816	-0.4102072704
3		-0.06254943848	-0.1262329102	-0.3461816406
4		-0.06339168596	-0.1189891975	-0.3033352624

In Table 2, we numerically show the energy eigenvalues of this potential at a fixed n by varying l for various screening parameters, $\delta_0 = 0.05, 0.075,$ 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.

Table 2. Energy bound states (eV) for the class of inversely quadratic Yukawa plus Hulthén potential with $\hbar = \mu = 1$ $V_{01}=2, V_{11}=-3, V_{21}=-3, V_{31}=0.05$

n	l	$\delta_0 = 0.05$	$\delta_0 = 0.075$	$\delta_0 = 0.1$
0	0	-4.455000000	-3.541805556	-3.145000000
	1	-1.215078125	-1.058752170	-1.035312500
	2	-0.6187500000	-0.6122492285	-0.6722222222
	3	-0.4197070312	-0.4794536676	-0.5882031250
	4	-0.3398000000	-0.44627222222	-0.6002000000
1	0	-1.247578125	-1.0975021700	-1.0778125000
	1	-0.6426388889	-0.6354436729	-0.6900000000
	2	-0.4337695312	-0.4853130426	-0.5788281250
	3	-0.3450000000	-0.4359722222	-0.5650000000
	4	-0.3073003472	-0.4341148245	-0.6028125000
2	0	-0.6550000000	-0.6479783951	-0.7005555555
	1	-0.4439257812	-0.4909771051	-0.5757031250
	2	-0.3499500000	-0.4306097222	-0.5428000000
	3	-0.3063281250	-0.4166495467	-0.5600347222
	4	-0.2896938776	-0.4312613379	-0.6123469388
3	0	-0.4492382812	-0.4943364801	-0.5750781250
	1	-0.3537500000	-0.4281597222	-0.5300000000
	2	-0.3063281250	-0.4051912134	-0.5308680556
	3	-0.2850000000	-0.4094756236	-0.5650000000
	4	-0.2803173828	-0.4340235731	-0.6267382812
4	0	-0.3558000000	-0.4272722222	-0.5242000000
	1	-0.3066753472	-0.3983335745	-0.5128125000
	2	-0.2820153061	-0.3943416950	-0.5316326531
	3	-0.2732080078	-0.4094337294	-0.5764257812
	4	-0.2759876543	-0.4406395748	-0.6450000000

In Table 3, we numerically present energy eigenvalues of Hulthén potential at 2p, 3p, 3d, 4p. As the screening parameter increases, the energy eigenvalues increase with increase in the quantum numbers. We compared our result for the Hulthén potential with the results from three other methods.

Using the energy equation found in Eq. (18), we quantitatively presented the eigenvalues for four diatomic molecules in Tables 4. The model parameters for each molecule listed in Table 4 were entered to do this. These diatomic molecules were chosen due to their significance in chemical physics and chemistry. In addition, we have also used the following

transformations: 1 amu = 931.494028 MeV/c^2 and $\hbar c = 1973.29$ eV $\mathring{\text{A}}$ [47-49]. The results show that the bound state energy spectra of these diatomic molecules increase as various quantum numbers n and l increases. Our newly developed potential models reduce to special cases by applying certain boundary conditions to validate the mathematical accuracy of our analytical calculations.

Table 3. Energy bound states (eV) of the Hulthén potential as a function of the screening parameters δ_0 for 2p, 3p, 3d, and 4p states and for $Z = 1$ in atomic units $(\hbar = \mu = e = 1)$.

State	δ_0	Present (NU)	AIM [43]	EQR [44]	SUSY [45]
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 diatomic molecules used in this work [50,51]

Molecule	$\delta_0 = \left(\mathring{\text{A}}\right)^{-1}$	$\mu(\text{amu})$	$\mu(\text{eV})$
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 Yukawa plus Hulthén potential $(V_{01} = 1,\ V_{11} = V_{21} = -1, V_{31} = 0.025)$ 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
	1	-30.30849598	-9.453142109	-36.45622154	-8.798919265
	2	-16.95021661	-6.930212578	-19.79018435	-6.641819365
	3	-12.30628452	-6.063890161	-13.98924338	-5.905643942
	4	-10.18475382	-5.679164767	-11.33218294	-5.583549884
	5	-9.059727937	-5.486789797	-9.915958908	-5.427786332
1	0	-30.07202715	-9.368846178	-36.19627464	-8.713879144
	1	-16.73132841	-6.849755612	-19.55063368	-6.559784975
	2	-12.11100219	-5.989268264	-13.77677931	-5.828574813
	3	-10.00628951	-5.607970361	-11.13933831	-5.509021515
	4	-8.892132746	-5.416928527	-9.736182578	-5.353695279
	5	-8.247963204	-5.317833657	-8.917746069	-5.278508861
2	0	-16.62260878	-6.809987732	-36.19627464	-6.519304712
	1	-11.98217237	-5.940383964	-19.55063368	-5.778202139
	2	-9.874266958	-5.555735276	-13.77677931	-5.454478305
	3	-8.760230009	-5.362421323	-11.13933831	-5.296033229
	4	-8.116182734	-5.261007963	-9.736182578	-5.217664321
	5	-7.724662434	-5.210441659	-8.917746069	-5.184264747
3	0	-11.91816497	-5.916200905	-13.56670214	-5.753317826
	1	-9.787121287	-5.521464611	-10.90210156	-5.418760482
	2	-8.662570784	-5.322346977	-9.489446311	-5.253726320

n	l	N_2	O_2	NO	CO
	3	-8.012355153	-5.216562617	-8.666361658	-5.170172128
	4	-7.616127092	-5.162076555	-8.158300703	-5.132017704
	5	-7.369538341	-5.139134138	-7.835113863	-5.122355833
4	0	-9.743809264	-5.504495097	-10.85516342	-5.401094865
	1	-8.598068359	-5.296014583	-9.420011074	-5.225969157
	2	-7.935415930	-5.183820812	-8.584125641	-5.135243324
	3	-7.530521367	-5.124161742	-8.067455968	-5.091126140
	4	-7.276939786	-5.096569587	-7.737532584	-5.076003205
	5	-7.119236710	-5.090491185	-7.525275330	-5.080827207

4. CONCLUSION

The Greene-Aldrich approximation scheme has been used to study the bound state solutions to the Schrödinger equation with the newly proposed potential of a class of inversely quadratic Yukawa plus Hulthén potential model. Using the NU technique, the eigenvalues and normalized eigenfunctions are determined. After that, we impute the experimental values for each molecular parameter and apply the solution for four diatomic molecules. The findings demonstrate that these diatomic molecules' bound state energy spectrum increases as various quantum numbers increase. These findings can be applied in Molecular and Chemical Physics.

Funding. Not applicable.
Conflicts of interest/Competing interests. The authors declare that they have no competing interests.
Code availability. Not applicable.
Authors contributions. EPI conceived and designed the study, acquired, analyzed, and interpreted the data, and handled the review; FOF handled the computational analysis, writing review, and editing. All authors read and approved the final manuscript.

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REFERENCES

[1] E.P. Inyang, E.O. Obisung, J. Amajama, E.S William, and I.B. Okon, "The Effect of Topological Defect on the Mass Spectra of Heavy and Heavy-Light Quarkonia," Eurasian Physical Technical Journal, **19**(4), 78-87 (2022). https://doi.org/10.31489/2022No4/78-87
[2] E.S. William, E.P. Inyang, I.O. Akpan, J.A. Obu, A.N. Nwachukwu, and E.P. Inyang, "Ro-vibrational energies and expectation values of selected diatomic molecules via Varshni plus modified Kratzer potential model," Indian Journal of Physics, **96**, 34613476 (2022). https://doi.org/10.1007/s12648-022-02308-0
[3] E.P. Inyang, E.P. Inyang, I.O. Akpan, J.E. Ntibi, and E.S. William, Masses and thermodynamic properties of a Quarkonium system. Canadian Journal of Physics. 99(11), 982-990 (2021). https://doi.org/10.1139/cjp-2020-0578
[4] I.B. Okon, C.A. Onate, R. Horchani, O.O. Popoola, E. Omugbe, E.S. William, U.S. Okorie, *et al*., "Thermomagnetic properties and its effects on Fisher entropy with Schioberg plus Manning-Rosen potential (SPMRP) using Nikiforov-Uvarov functional analysis (NUFA) and supersymmetric quantum mechanics (SUSYQM) methods," Scientifc Reports, 13, 8193 (2023). https://doi.org/10.1038/s41598-023-34521-0
[5] F. Ayedun, E.P. Inyang, E.A. Ibanga, and K.M. Lawal, "Analytical Solutions to The Schrödinger Equation with Collective Potential Models: Application to Quantum Information Theory," East Eur. J. Phys. **4**, 87-98 (2022). https://doi.org/10.26565/2312-4334-2022-4-06
[6] E.S. William, S.C. Onye, A.N. Ikot, A.N. Nwachukwu, E.P. Inyang, I.B. Okon, I.O. Akpan and B. I. Ita, "Magnetic susceptibility and Magnetocaloric effect of Frost-Musulin potential subjected to Magnetic and Aharonov-Bohm(Flux)for CO and NO diatomic molecules", Journal of Theoretical and Applied Physics, **17**, 1-12 (2023). https://doi.org/10.30495/JTAP.172318
[7] C. Berkdermir, A. Berkdemir, and R. Sever, "Polynomial solutions of the Schrodinger equation for the generalized Woods-Saxon potential," Phys. Rev. C, **72**, 027001 (2008). http://dx.doi.org/10.1103/PhysRevC.72.027001
[8] M. Abu-Shady, and E.P. Inyang, "The Fractional Schrödinger Equation with The Generalized Woods-Saxon Potential," East European Journal of Physics, **1**. 63-68 (2023). https://doi.org/10.26565/2312-4334-2023-1-06
[9] S.M. Ikhdair, "The bound state solutions of the Manning-Rosen potential including an improved approximation to the orbital centrifugal term," Phys. Scr. **83**, 015010 (2011). https://doi.org/10.1088/0031-8949/83/01/015010
[10] J. Lu, "Approximate spin and pseudospin solutions of the Dirac equation," Physica Scripta, **72**, 349 (2005). https://doi.org/10.1238/Physica.Regular.072a00349
[11] R.L. Greene, and C. Aldrich, "Variational wave functions for a screened Coulomb potential," Phys. Rev. A, **14**, 2363 (1976). https://doi.org/10.1103/PhysRevA.14.2363
[12] C.S. Jia, T. Chen, and L.G. Cui, "Approximate analytical solutions of the Dirac equation with the generalized Pöschl-Teller potential including the pseudo-centrifugal term," Phys. Lett. A, **373**, 1621-1626 (2009). https://doi.org/10.1016/j.physleta.2009.03.006
[13] E.L. Hill, "The Theory of Vector Spherical Harmonics," Am. J. Phys. **22**, 211-214 (1954). https://doi.org/10.1119/1.1933682
[14] C.L. Pekeris, "The Rotation-Vibration Coupling in Diatomic Molecules," Phys. Rev. **45**, 98 (1934). https://doi.org/10.1103/PhysRev.45.98
[15] B.H. Yazarloo, H. Hassanabadi, and S. Zarrinkamar, "Oscillator strengths based on the Mobius square potential under Schrodinger equation," Eur. Phys. J. Plus, **127**, 51 (2012). https://doi.org/10.1140/epjp/i2012-12051-9
[16] S.H. Dong, W.C. Qiang, G.H. Sun, and V.B. Bezerra, "Analytical approximations to the *l*-wave solutions of the Schrödinger equation with the Eckart potential," J. Phys. A, **40**, 10535 (2007). https://doi.org/10.1088/1751-8113/40/34/010

[17] S.K. Nikiforov, and V.B. Uvarov, *Special functions of Mathematical Physics*, (Birkhauser, Basel, 1988).
[18] E.S. William, E.P. Inyang, and E.A. Thompson, "Arbitrary ℓ -solutions of the Schrödinger equation interacting with Hulthén-Hellmann potential model," Rev. Mex. Fis. **66**, 730 (2020). https://doi.org/10.31349/RevMexFis.66.730
[19] I.O. Akpan, E.P. Inyang, E.P. Inyang, and E.S. William, "Approximate solutions of the Schrödinger equation with Hulthen-Hellmann Potentials for a Quarkonium system," Rev. Mex. Fis. **67**, 482-490 (2021). https://doi.org/10.31349/revmexfis.67.482
[20] E.P. Inyang, E.O. Obisung, E.S. William, and I.B. Okon, "Non-Relativistic study of mass spectra and thermal properties of a quarkonium system with Eckart-Hellmann potential," East European Journal of Physics, **3**, 104-114 (2022). https://doi.org/10.26565/2312-4334-2022-3-14
[21] E.P. Inyang, F.O. Faithpraise, J. Amajama, E.S. William, E.O. Obisung, and J.E. Ntibi, "Theoretical Investigation of Meson Spectrum using Exact Quantization Rule Technique," East European Journal of Physics, **1**, 53-62 (2023). https://doi.org/10.26565/2312-4334-2023-1-05
[22] A.N. Ikot, U.S. Okorie, P.O. Amadi, C.O. Edet, G.J. Rampho, and R. Sever, "The Nikiforov-Uvarov Functional Analysis (NUFA) Method: A new approach for solving exponential-Type potentials," Few-Body System, **62**, 9 (2021). https://doi.org/10.1007/s00601-021-021-01593-5
[23] C.O. Edet, S. Mahmoud, E.P. Inyang, N. Ali, S.A. Aljunid, R. Endut, A.N. Ikot, and M. Asjad, "Non-Relativistic Treatment of the 2D Electron System Interacting via Varshni-Shukla Potential Using the Asymptoptic Iteration Method," Mathematics, **10**, 2824 (2022). https://doi.org/10.3390/math10152824
[24] A.N. Ikot, L.F. Obagboye, U.S. Okorie, E.P. Inyang, P.O. Amadi, and A. Abdel-Aty, Solutions of Schrodinger equation with generalized Cornell potential (GCP) and its applications to diatomic molecular systems in D-dimensions using Extended Nikiforov–Uvarov (ENU) formalism," The European Physical Journal Plus, 137, 1370 (2022). https://doi.org/10.1140/epjp/s13360-022-03590-x
[25] E.O. Omugbe, E. Osafile, E.P. Inyang, and A. Jahanshir, "Bound state solutions of the hyper-radial Klein-Gordon equation under the Deng-Fan potential by WKB and SWKB methods," Physica Scripta, **96**, 125408 (2021). https://doi.org/10.1088/1402-4896/ac38d4
[26] E.S. William, E.P. Inyang, J.E. Ntibi, J.A. Obu, and E.P. Inyang, "Solutions of the Non-relativistic Equation Interacting with the Varshni-Hellmann potential model with some selected Diatomic molecules," Jordan Journal of Physics, **15**, 179-193 (2022). https://doi.org/10.47011/15.2.8
[27] M. Abu-Shady, and E.P. Inyang, "Heavy-Light Meson masses in the Framework of Trigonometric Rosen-Morse Potential using the Generalized Fractional Derivative," East Eur. J. Phys. **4**, 80-87 (2022). https://doi.org/10.26565/2312-4334-2022-4-06
[28] B.I. Ita, "Solutions of the Schrödinger equation with inversely quadratic Hellmann plus Mie-type potential using Nikiforov-Uvarov method," International Journal of Recent Advances in Physics. **2**(4), 25 (2013). https://wireilla.com/physics/ijrap/papers/2413ijrap02.pdf
[29] B.I. Ita, and A.I. Ikeuba, "Solutions to the Schrödinger Equation with Inversely Quadratic Yukawa Plus Inversely Quadratic Hellmann Potential Using Nikiforov-Uvarov Method," Phys. Journal of Atomic and Molecular Physics, 582610 (2013). https://doi.org/10.1155/2013/582610
[30] E.P. Inyang, E.S. William, J.O. Obu, B.I. Ita, E.P. Inyang, and I.O. Akpan, "Energy spectra and expectation values of selected diatomic molecules through the solutions of Klein-Gordon equation with Eckart-Hellmann potential model," Molecular Physics, **119**(23), e1956615 (2021). https://doi.org/10.1080/00268976.2021.1956615
[31] B.I. Ita, C.O. Ehi-Eromosele, A. Edobor-Osoh, and A.I. Ikeuba, "Solutions of the Schrödinger equation with inversely quadratic Hellmann plus inversely quadratic potential using Nikiforov-Uvarov method," AIP Conf. Proc. **1629**, 360 (2014). https://doi.org/10.1063/1.4902294
[32] K.J. Oyewumi, and E.A. Bangudu, "Isotropic harmonic oscillator plus inverse quadratic potential in N-dimensional spaces," Arab. J. Sci. Eng. **28**, 173-182 (2003).
[33] R.H. Parmar, K.R. Purohit, and A.K. Rai, "Approximaate analytical solution of the extended Hulthen-Yukawa with inverse square and Coulombic term plus ring shape potential," AIP Conf. Proc. **2220**, 140071 (2020). https://doi.org/10.1063/5.0001432
[34] B.I. Ita, N. Nzeata-Ibe, T.O. Magu, and L. Hitler, "Bound-State Solutions of the Schrödinger Equation with Woods–Saxon Plus Attractive Inversely Quadratic Potential via Parametric Nikiforov-Uvarov Method," Manila Journal of Science, **11**, 58-67 (2018). https://www.dlsu.edu.ph/wp-content/uploads/pdf/research/journals/mjs/MJS11-2018/volume-1/MJS11-6-Ita-et-al.pdf
[35] A. Maireche, "New Exact Non-Relativistic Energy Eigen Values for Modified Inversely Quadratic Hellmann Plus Inversely Quadratic Potential," J. Nanosci. Curr. Res. **2**, 1000115 (2017). https://doi.org/10.4172/2572-0813.1000115
[36] L. Hulthen, "Über die eigenlosunger der Schrödinger-Gleichung des deuterons," Ark. Mat. Astron. Fys. A, **28**, 5 (1942).
[37] E.P. Inyang, E.S. William, E. Omugbe, and F. Ayedun, "The study of H_2 and N_2 Diatomic Molecules in Arbitrary Dimensions with Collective Potential Model," Bulgarian Journal of Physics, **50**, 1-15 (2023). https://www.bjp-bg.com/papers/bjp1578.pdf
[38] I.B. Okon, O. Popoola, and E.E. Ituen, "Bound state solution to Schrödinger equation with Hulthen plus exponential Coulombic potential with centrifugal potential barrier using parametric Nikiforov Uvarov method," Intl. J. Rec. adv. Phys. **5**, 5101 (2016). https://doi.org/10.14810/ijrap.2016.5101
[39] E.P. Inyang, J. Ntibi, E.A. Ibanga, F. Ayedun, E.P. Inyang, and E.S. William, "Thermal Properties, Mass Spectra and Root Mean Square Radii of Heavy Quarkonium System with Class of Inversely Quadratic Yukawa Potential," AIP Conference Proceedings 2679, 030003 (2023). https://doi.org/10.1063/5.0112829
[40] E.S. William, I.B. Okon, O.O. Ekerenam, I.O. Akpan, B.I. Ita, E.P. Inyang, I.P. Etim, and I.F. Umoh, "Analyzing the effects of magnetic and Aharonov-Bohm (AB) flux fields on the energy spectra and thermal properties of N_2, NO, CO, and H_2 diatomic molecules," International Journal of Quantum Chemistry, (2022). https://doi.org/10.1002/qua.26925
[41] O. Bayrak, G. Kocak, and I. Boztosun, "Any *l*-state solutions of the Hulth´en potential by the asymptotic iteration method, J. Phys. A, **39**, 11521 (2006). https://doi.org/10.1088/0305-4470/39/37/012
[42] I.B. Okon, and O. Popoola, "Bound-State solution of Schrodinger equation with Hulthen plus generalized exponential Coulomb potential using Nikiforov-Uvarov method," Intl. J. Rec. Adv. Phys. **4**(3), 1-12 (2015). https://doi.org/10.14810/ijrap.2015.4301
[43] K.J. Oyewumi, and O.J. Oluwadare, "The scattering phase shifts of the Hulthen-type potential plus Yukawa potential," Eur. Phys. J. Plus, **131**, 295 (2016). https://doi.org/10.1140/epjp/i2016-16295-y

[44] W.C. Qiang, Y. Gao, and R. Zhou, "Arbitrary *l*-state approximate solutions of the Hulthen potential through the exact quantization rule," Cen. Eur. Phys. J. Phys. **6**, 356 (2008). https://doi.org/10.2478/s11534-008-0041-1
[45] S.M. Ikhdair, "An improved approximation scheme for the centrifugal term and the Hulth´en potential, The Eur. Phys. J. A, **39**, 307 (2009). https://doi.org/10.1140/epja/i2008-10715-2
[46] L. Hitler, B.I. Ita, P.A. Isa, N. Nzeata-Ibe, I. Joseph, O. Ivan, and T.O. Magu, "Wkb Solutions for Inversely Quadratic Yukawa plus Inversely Quadratic Hellmann Potential," World Journal of Applied Physics, **2**, 4 (2017). https://article.sciencepublishinggroup.com/pdf/10.11648.j.wjap.20170204.13.pdf
[47] E.P. Inyang, E.S. William, J.E. Ntibi, J.A. Obu, P.C. Iwuji, and E.P. Inyang, "Approximate solutions of the Schrödinger equation with Hulthén plus screened Kratzer Potential using the Nikiforov-Uvarov – functional analysis (NUFA) method: an application to diatomic molecules," Can. J. Phys. **100**(10), 473 (2022). https://doi.org/10.1139/cjp-2022-003
[48] E.P. Inyang, I.B. Okon, F.O. Faithpraise, E.S. William, P.O. Okoi, and E.A. Ibanga, "Quantum mechanical treatment of Shannon entropy measure and energy spectra of selected diatomic molecules with the modified Kratzer plus generalized inverse quadratic Yukawa potential model," Journal of Theoretical and Applied Physics, **17**(4), (2023). https://doi.org/10.57647/J.JTAP.2023.1704.40
[49] E.P. Inyang, F. Ayedun, E.A. Ibanga, K.M. Lawal, I.B. Okon, E.S. William, O. Ekwevugbe, *et al*., "Analytical Solutions of the N-Dimensional Schrödinger equation with modified screened Kratzer plus Inversely Quadratic Yukawa potential and Thermodynamic Properties of selected Diatomic Molecules," Results in Physics, **43**, 106075 (2022). https://doi.org/10.1016/j.rinp.2022.106075
[50] E.P. Inyang, E.S. William, J.E. Ntibi, J.A. Obu, P.C. Iwuji, and E.P. Inyang, "Approximate solutions of the Schrodinger equation with Hulthen plus screened Kratzer potential using the Nikiforov-Uvarov-Functional analysis method: An Application to diatomic molecules," Canadian Journal of Physics, **100**(10), 463-473 (2022). https://doi.org/10.1139/cjp-2022-0030
[51] K.J. Oyewumi, and K.D. Sen, "Exact solutions of the Schrödinger equation for the pseudoharmonic potential: an application to some diatomic molecules," J. Math. Chem. **50**, 1039-1059 (2012). https://doi.org/10.1007/s10910-011-9967-4

ВЛАСНІ ЗНАЧЕННЯ ЗВ'ЯЗАНОГО СТАНУ ТА КОЛИВАЛЬНОЇ ЕНЕРГІЇ ВИБРАНИХ ДВОХАТОМНИХ МОЛЕКУЛ З КЛАСОМ ОБЕРНЕНО КВАДРАТИЧНОЇ МОДЕЛІ ЮКАВИ ПЛЮС ПОТЕНЦІАЛ ХУЛЬТХЕНА

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В цьому дослідженні для розв'язання рівняння Шредінгера використовується підхід Нікіфорова-Уварова з використанням класу обернено квадратичної моделі Юкави плюс потенціалу Хультена з наближенням до відцентрового члена. Отримано нормовану хвильову функцію та рівняння власних значень енергії. Чисельний зв'язаний стан для кількох двоатомних молекул (N_2, O_2, NO та CO) для різних обертальних і вібраційних квантових чисел було розраховано за допомогою енергетичного рівняння та відповідних спектроскопічних даних. Наші результати показують, що за відсутності розбіжності між s-хвилею та *l*-хвилею власні значення енергії дуже чутливі до потенціалу та властивостей двохатомної молекули, що свідчить про те, що підхід наближення підходить для цього набору потенціалів. Результати узгоджуються з попередніми дослідженнями в літературі, і ми також знайшли чотири особливі випадки цього потенціалу.

Ключові слова: *рівняння Шредінгера; метод Нікіфорова-Уварова; клас обернено квадратичного плюс потенціал Хюльтена; двохатомні молекули; зв'язаний стан*