

The study of H₂ and N₂ Diatomic Molecules in Arbitrary Dimensions with Collective Potential Model

Etido P. Inyang^{1*}, Eddy S. William², Ekwevugbe Omugbe³, Funmilayo Ayedun¹

¹Department of Physics, National Open University of Nigeria, Jabi-Abuja, Nigeria

²Theoretical Physics Group, Department of Physics, School of Pure and Applied Sciences, Federal University of Technology, Ikot Abasi, Nigeria

³Department of Physics, University of Agriculture and Environmental Sciences, Umuagwo, Imo State, Nigeria

*Corresponding author's E-mail: etidophysics@gmail.com

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Abstract. The analytical bound state solution of the Schrödinger equation with the collective potential model (Hulthén plus screened Kratzer potential) is solved using the Nikiforov-Uvarov-Functional Analysis (NUFA) method. We obtain the energy equation and the wave function with the Greene-Aldrich approximation scheme to the centrifugal term in closed form. The numerical energy eigenvalues and expectation values using Hellmann–Feynman theorem for Hydrogen and Nitrogen diatomic molecules were computed for various quantum states. We also computed the bound state energy of Hulthén potential and our results are consistent with the reports in the literature. The special case energy equations obtained from the NUFA method were the same when compared to other analytical methods, and this validate a high level of mathematical precision of our method.

KEY WORDS: Energy spectra; expectation values; Nikiforov-Uvarov-functional analysis method; Hulthén-screened Kratzer potential; diatomic molecules.

1 Introduction

The solution of the Schrodinger equation (SE) is vital in the study of the dynamics of the non-relativistic particles in quantum mechanics such as, the thermodynamic properties (TP) of the system, mass spectra of mesons, among others [1–5]. Its solutions with diverse potential functions have been investigated

by many authors [6–20]. Also, different techniques have been employed in obtaining the solutions of the Schrodinger equation such as, asymptotic iteration method [21], Laplace transformation method [22], super symmetric quantum mechanics [23], the Nikiforov-Uvarov method [24], the Nikiforov-Uvarov Functional Analysis (NUFA) method [25], the series expansion method [26], the extended Nikiforov-Uvarov method [27], the WKB approximation method [28] and so on.

Recently, many scholars have devoted interest in investigating bound state energy of various diatomic molecules (DMs) with a single potential function and a collective potential function [29–37]. For instance, Inyang et al. [38] combined Eckart and Hellmann potential function to study some selected diatomic molecules. Also, Obogo et al. [39], investigated some selected diatomic molecules with q-deformed Hulthén quadratic exponential-type potential. In addition, Edet and Ikot [40] studied some diatomic molecules with the shifted Deng-Fan potential. Furthermore, Edet et al. [41] computed the energy spectra of some diatomic molecules with Deng-Fan plus Eckart potential. Motivated by the success of other researchers, we seek to combine Hulthén plus screened Kratzer potentials (HSKP) to study some selected diatomic molecules through the solutions of the SE using the NUFA method. The Hulthén potential (HP) [42] is crucial in exploring the interaction existing between two particles. It is applied in nuclear and molecular physics, atomic physics, etc. [43, 44].

On the other hand, Ikot et al. [45] proposed the screened Kratzer potential (SKP) which, finds application in molecular physics, and many authors have employed in literature [46–49].

The aim of this study is to obtain the solutions to the SE with the Hulthén plus screened Kratzer potential model and apply it to study energy spectra and expectation values using Hellmann–Feynman theorem of the Hydrogen (H_2) and Nitrogen (N_2) diatomic molecules. The essence of combining at least two potential functions is to have a better result, because potential with more fitting parameters tends to give a better results output [50]. The collective potential reads:

$$V(r) = -\frac{V_0 e^{-\vartheta r}}{1 - e^{-\vartheta r}} - \frac{V_1 e^{-\vartheta r}}{r} + \frac{V_2 e^{-\vartheta r}}{r^2}, \quad (1)$$

where V_0 is the potential strength for Hulthén, ϑ is the screening parameter. The letter $V_1 \equiv 2D_e r_e$ and $V_2 \equiv D_e r_e^2$, here D_e is the dissociation energy and r_e is the equilibrium bond length.

2 Review of Nikiforov-Uvarov-Functional Analysis (NUFA) Method

The NUFA method proposed recently by Ikot et al. [25] is a simple method for solving a second order differential equation. This method is a combination of

the NU [24], parametric NU [51], and factorization [52] methods.

$$\psi''(y) + \frac{\tilde{\tau}(y)}{\sigma(y)}\psi'(y) + \frac{\tilde{\sigma}(y)}{\sigma^2(y)}\psi(y) = 0, \quad (2)$$

where $\tilde{\sigma}(y)$ and $\sigma(y)$ are polynomials of second degree and $\tilde{\tau}(y)$ is a polynomial of first degree. Tezcan and Sever [51] latter introduced the parametric form of the NU method in the form

$$\psi'' + \frac{\beta_1 - \beta_2 y}{y(1 - \beta_3 y)}\psi' + \frac{1}{y^2(1 - \beta_3 y)^2}[-\xi_1 y^2 + \xi_2 y - \xi_3]\psi(y) = 0, \quad (3)$$

where β_i and ξ_i ($i = 1, 2, 3$) are all parameters. From Eq. (3) at $y \rightarrow 0$ and $y \rightarrow 1$, we take the wave function as,

$$\psi(y) = y^\lambda (1 - y)^v f(y). \quad (4)$$

Replacing Eq. (4) into Eq. (3) is as follows:

$$\begin{aligned} & y(1 - \beta)y''(y) + [\beta_1 + 2\lambda - (2\lambda\beta_3 + 2v\beta_3 + \beta_2)y]f'(y) \\ & - \beta_3 \left(\lambda + v + \frac{\beta_2}{\beta_3} - 1 + \sqrt{\left(\frac{\beta_2}{\beta_3} - 1\right)^2 + \frac{\xi_1}{\beta_3}} \right) \\ & \times \left(\lambda + v + \frac{\beta_2}{\beta_3^2} - 1 + \sqrt{\left(\frac{\beta_2}{\beta_3} - 1\right)^2 + \frac{\xi_1}{\beta_3^2}} \right) \\ & + \left[\frac{\lambda(\lambda - 1) + \beta_1\lambda - \xi_3}{y} \right. \\ & \left. + \frac{\beta_2 v - \beta_1\beta_3 v + v(v - 1)\beta_3 - \frac{\xi_1}{\beta_3} + \xi_2 - \xi_3\beta_3}{(1 - \beta_3 y)} \right] f(y) = 0. \quad (5) \end{aligned}$$

Equation (5) is reduced to a Gauss hypergeometric equation when following functions is zero:

$$\lambda(\lambda - 1) + \beta_1\lambda - \xi_3 = 0, \quad (6)$$

$$\beta_2 v - \beta_1\beta_3 v + v(v - 1)\beta_3 - \frac{\xi_1}{\beta_3} + \xi_2 - \xi_3\beta_3 = 0. \quad (7)$$

Thus Eq. (5) becomes

$$\begin{aligned} & y(1 - \beta_1 y)f''(y) + [\beta_1 + 2\lambda - (2\lambda\beta_3 + 2v\beta_3 + \beta_2)y]f'(y) \\ & - \beta_3 \left(\lambda + v + \frac{\beta_2}{\beta_3} - 1 + \sqrt{\left(\frac{\beta_2}{\beta_3} - 1\right)^2 + \frac{\xi_1}{\beta_3}} \right) \\ & \times \left(\lambda + v + \frac{\beta_2}{\beta_3^2} - 1 + \sqrt{\left(\frac{\beta_2}{\beta_3} - 1\right)^2 + \frac{\xi_1}{\beta_3^2}} \right) f(y) = 0. \quad (8) \end{aligned}$$

Solving Eqs. (6) and (7) gives Eqs. (9) and (10),

$$\lambda = \frac{(1 - \beta_1)}{2} \pm \frac{1}{2} \sqrt{(1 - \beta_1)^2 + 4\xi_3} \quad (9)$$

$$v = \frac{(\beta_3 + \beta_1\beta_3 - \beta_2) \pm \sqrt{(\beta_3 + \beta_1\beta_3 - \beta_2)^2 + \left(\frac{\xi_1}{\beta_3} + \beta_3\xi_3 - \xi_2\right)}}{2}. \quad (10)$$

Equation (8) is the hyper geometric equation type of the form

$$y(1 - y)f''(y) + [c + (a + b + 1)y]f'(y) - abf(y) = 0. \quad (11)$$

Using Eqs. (4), (8) and (11), we obtain the energy equation and the corresponding wave equation respectively for the NUFA method as follows:

$$\begin{aligned} \lambda^2 + 2\lambda\left(v + \frac{\beta_2}{\beta_3} - 1 + \frac{n}{\sqrt{\beta_3}}\right) + \left(v + \frac{\beta_2}{\beta_3} - 1 + \frac{n}{\sqrt{\beta_3}}\right)^2 \\ - \left(\frac{\beta_2}{\beta_3} - 1\right)^2 - \frac{\xi_1}{\beta_3^3} = 0, \end{aligned} \quad (12)$$

$$\begin{aligned} \psi(y) = N_y \frac{(1 - \beta_1) + \sqrt{(1 - \beta_1)^2 + 4\xi_3}}{2} (1 - \beta_3 y) \\ \times \frac{(\beta_3 + \beta_1\beta_3 - \beta_2) \pm \sqrt{(\beta_3 + \beta_1\beta_3 - \beta_2)^2 + \left(\frac{\xi_1}{\beta_3} + \beta_3\xi_3 - \xi_2\right)}}{2} \\ \times {}_2F_1(a, b, c; y), \end{aligned} \quad (13)$$

where a , b , and c are given as follows;

$$a = \sqrt{\beta_3} \left(\lambda + v + \frac{\beta_2}{\beta_3} - 1 + \sqrt{\left(\frac{\beta_2}{\beta_3} - 1\right)^2 + \frac{\xi_1}{\beta_3}} \right), \quad (14)$$

$$b = \sqrt{\beta_3} \left(\lambda + v + \frac{\beta_2}{\beta_3} - 1 - \sqrt{\left(\frac{\beta_2}{\beta_3} - 1\right)^2 + \frac{\xi_1}{\beta_3}} \right), \quad (15)$$

$$c = \beta_1 + 2\lambda. \quad (16)$$

3 Solutions of the Schrödinger Equation with the Collective Potential Model (Hulthén Plus Screened Kratzer Potential)

The Schrödinger equation takes the form [53]

$$\frac{d^2\psi(r)}{dr^2} + \left[\frac{2\mu}{\hbar^2} (E_{nl} - V(r)) - \frac{l(l+1)}{r^2} \right] \psi(r) = 0, \quad (17)$$

where μ is the reduced mass, \hbar is the reduced Planck constant and r is the radial distance.

To solve Eq. (17), the Greene-Aldrich approximation [54] is introduced to deal with the centrifugal obstacle and is valid for $\vartheta \ll 1$, and it reads

$$\frac{1}{r^2} \approx \frac{\vartheta^2}{(1 - e^{-\vartheta r})^2}. \quad (18)$$

Replacing Eqs. (1) and (18) into Eq. (17), Eq. (19) is obtained as

$$\begin{aligned} \frac{d^2\psi(r)}{dr^2} + \left[\frac{2\mu E_{nl}}{\hbar^2} + \frac{2\mu V_0 e^{-\vartheta r}}{\hbar^2(1 - e^{-\vartheta r})} + \frac{2\mu V_1 \vartheta e^{-\vartheta r}}{\hbar^2(1 - e^{-\vartheta r})} \right. \\ \left. - \frac{2\mu V_2 \vartheta^2 e^{-\vartheta r}}{\hbar^2(1 - e^{-\vartheta r})^2} - \frac{\vartheta^2 l(l+1)}{(1 - e^{-\vartheta r})^2} \right] \psi(r) = 0. \end{aligned} \quad (19)$$

We set,

$$y = e^{-\vartheta r}. \quad (20)$$

Differentiating Eq. (20), we have Eq. (21) as

$$\frac{d^2\psi(r)}{dr^2} = \vartheta^2 y^2 \frac{d^2\psi(y)}{dy^2} + \vartheta^2 y \frac{d\psi(y)}{dy}. \quad (21)$$

Putting Eqs. (20) and (21) into Eq. (19) and after some simplifications, we have

$$\begin{aligned} \frac{d^2\psi(y)}{dy^2} + \frac{1-y}{y(1-y)} \frac{d\psi(y)}{dy} \\ + \frac{1}{y^2(1-y)^2} [-(\varepsilon + \eta_0)y^2 + (2\varepsilon + \eta_0 - \eta_1)y - (\varepsilon + \gamma)] \psi(y) = 0, \end{aligned} \quad (22)$$

where

$$-\varepsilon = \frac{2\mu E_{nl}}{\vartheta^2 \hbar^2}, \quad \eta_0 = \frac{2\mu V_0}{\vartheta^2 \hbar^2} + \frac{2\mu V_1}{\vartheta \hbar^2}, \quad \eta_1 = \frac{2\mu V_2}{\hbar^2}, \quad \gamma = l(l+1). \quad (23)$$

Linking Eq. (22) and Eq. (3), gives

$$\beta_1 = \beta_2 = \beta_3 = 1, \quad \xi_1 = \varepsilon - \eta_0, \quad \xi_2 = 2\varepsilon + \eta_0 - \eta_1, \quad \xi_3 = \varepsilon + \gamma. \quad (24)$$

Inserting Eq. (24) into Eqs. (9) and (10), we have

$$\lambda = \frac{1}{2} \sqrt{4(\varepsilon + \gamma)}, \quad (25)$$

$$v = \frac{1 + \sqrt{1 + 4(\eta_1 + \gamma)}}{2}. \quad (26)$$

Plugging Eqs. (23), (24), (25) and (26) into Eq. (12), we obtain the energy equation of the Hulthén plus screened Kratzer potential as

$$E_{nl} = \frac{\vartheta^2 \hbar^2 l(l+1)}{2\mu} - \frac{\vartheta^2 \hbar^2}{8\mu} \left\{ \left[\left(n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2} \right)^2 + \frac{2\mu D_e r_e^2}{\hbar^2}} \right)^2 - \frac{2\mu V_0}{\vartheta^2 \hbar^2} + \frac{4\mu D_e r_e}{\hbar^2 \vartheta} + l(l+1) \right] \times \left(n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2} \right)^2 + \frac{2\mu D_e r_e^2}{\hbar^2}} \right)^{-1} \right\}^2. \quad (27)$$

Inserting Eq. (24) into Eq. (13), the wave function is given as

$$\psi(y) = N \frac{\sqrt{4(\varepsilon + \gamma)}}{2} \times (1-y) \frac{1 + \sqrt{1 + \eta_1 + \gamma}}{2} {}_2F_1(a, b, c; y), \quad (28)$$

where

$$a = \frac{1}{2} \sqrt{4(\varepsilon + \gamma)} + \frac{1 + \sqrt{1 + 4(\eta_1 + \gamma)}}{2} + \sqrt{\varepsilon + \eta_0}, \quad (29)$$

$$b = \frac{1}{2} \sqrt{4(\varepsilon + \gamma)} + \frac{1 + \sqrt{1 + 4(\eta_1 + \gamma)}}{2} - \sqrt{\varepsilon + \eta_0}, \quad (30)$$

$$c = 1 + \sqrt{4(\varepsilon + \gamma)} \quad (31)$$

Special cases of Hulthén plus screened Kratzer potential

1. In the case $V_1 = V_2 = 0$, we have the Hulthén potential of Eq. (32) and its energy equation of Eq. (33)

$$V(r) = -\frac{V_0 e^{-\vartheta r}}{1 - e^{-\vartheta r}}, \quad (32)$$

$$E_{nl} = \frac{\vartheta^2 \hbar^2 l(l+1)}{2\mu} - \frac{\vartheta^2 \hbar^2}{8\mu} \left[\frac{(n+l+1)^2 - \frac{2\mu V_0}{\vartheta^2 \hbar^2} + l(l+1)}{n+l+1} \right]^2. \quad (33)$$

Equation (33) is in agreement with Eq. (32) of [14] and Eq. (37) of [15].

2. By setting $V_0 = 0$, we have the screened Kratzer potential of Eq.(34) and its energy equation of Eq. (35)

$$V(r) = -\frac{V_2 e^{-\vartheta r}}{r} + \frac{V_3 e^{-\vartheta r}}{r^2} \quad (34)$$

$$E_{nl} = \frac{\vartheta^2 \hbar^2 l(l+1)}{2\mu} - \frac{\vartheta^2 \hbar^2}{8\mu} \left[\frac{\left(n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2} \right)^2 + \frac{2\mu D_e r_e^2}{\hbar^2}} \right)^2 + \frac{4\mu D_e r_e}{\hbar^2 \vartheta} + l(l+1)}{n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2} \right)^2 + \frac{2\mu D_e r_e^2}{\hbar^2}}} \right]^2. \quad (35)$$

Equation (35) is in agreement with Eq. (29) of [45].

3. By setting $V_0 = \vartheta = 0$ we have the Kratzer potential (KP) of Eq. (36) and its energy equation of Eq. (37)

$$V(r) = -\frac{V_1}{r} + \frac{V_2}{r^2}, \quad (36)$$

$$E_{nl} = -\frac{2\mu D_e^2 r_e^2}{\hbar^2 \left(n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2} \right)^2 + \frac{2\mu D_e r_e^2}{\hbar^2}} \right)^2} \quad (37)$$

Equation (37) agrees with Eq. (29) of [45];

4 The Expectation Values of the Collective Potential Model Hulthén plus Screened Kratzer Potential) Using the Hellmann–Feynman Theorem

The Hellmann–Feynman theorem (HFT) [55–57] is used in obtaining expectation values of some quantum mechanical observables for any arbitrary values of quantum numbers. Let \hat{H} be Hamiltonian of some parameter q . Let $E(q)$ and $\Psi(q)$ be the eigenvalues and the eigenfunctions of the Hamiltonian $\hat{H}(q)$. Then, the HFT states that

$$\frac{\partial E_{nl}(q)}{\partial q} = \langle \psi_{nl}(q) | \frac{\partial \hat{H}(q)}{\partial q} | \psi_{nl}(q) \rangle. \quad (38)$$

The effective Hamiltonian is given as

$$\hat{H} = -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} - \frac{\hbar^2}{\mu r} \frac{d}{dr} + \frac{\hbar^2}{2\mu r^2} l(l+1) - \frac{V_0 e^{-\vartheta r}}{1 - e^{-\vartheta r}} - \frac{V_1 e^{-\vartheta r}}{r} + \frac{V_2 e^{-\vartheta r}}{r^2}. \quad (39)$$

4.1 Expectation value of $\langle r^{-2} \rangle$

Substituting $q = l$ into Eq. (38) gives

$$\frac{\partial E_{nl}(l)}{\partial l} = \langle \psi_{nl}(l) | \frac{\partial \hat{H}(l)}{\partial l} | \psi_{nl}(l) \rangle. \quad (40)$$

Partial derivative of Eq. (39) with respect to l gives

$$\langle \psi(l) \left| \frac{\partial H(l)}{\partial l} \right| \psi(l) \rangle = \frac{\hbar^2}{2\mu} (2l+1) \langle r^{-2} \rangle. \quad (41)$$

Partial derivative of Eq. (27) with respect to l gives

$$\begin{aligned} \frac{\partial E_{nl}(l)}{\partial l} = & \frac{\vartheta \hbar^2}{2\mu} (2l+1) - 2BV \left\{ \frac{1}{2\sqrt{F}} - \left[\left(n + \frac{1}{2} + \sqrt{F} \right) (2l+1) \right. \right. \\ & \left. \left. + \left(\frac{2V_0\mu}{\hbar^2\vartheta^2} + \frac{4\mu D_e r_e}{\hbar^2\vartheta} + l(l+1) \right) \frac{1}{2\sqrt{F}} (2l+1) \right] \left(n + \frac{1}{2} + \sqrt{F} \right)^{-2} \right\}, \end{aligned} \quad (42)$$

where

$$B = \frac{\hbar^2\vartheta^2}{8\mu}, \quad (43)$$

$$F = \left(l + \frac{1}{2} \right)^2 + \frac{2D_e r_e^2 \mu}{\hbar^2}, \quad (44)$$

$$V = \left(n + \frac{1}{2} + \sqrt{F} \right) - \frac{\frac{2\mu V_0}{\vartheta^2 \hbar^2} + \frac{4\mu D_e r_e}{\vartheta \hbar^2} + l(l+1)}{\left(n + \frac{1}{2} + \sqrt{F} \right)} \quad (45)$$

Connecting Eqs. (41) and (42) yields the expectation values of $\langle r^{-2} \rangle$. Hence,

$$\begin{aligned} \langle r^{-2} \rangle = & \vartheta - \frac{4\mu BV}{\hbar^2(2l+1)} \left\{ \frac{1}{2\sqrt{F}} - \left[\left(n + \frac{1}{2} + \sqrt{F} \right) (2l+1) \right. \right. \\ & \left. \left. + \left(\frac{2V_0\mu}{\hbar^2\vartheta^2} + \frac{4\mu D_e r_e}{\hbar^2\vartheta} + l(l+1) \right) \frac{1}{2\sqrt{F}} (2l+1) \right] \left(n + \frac{1}{2} + \sqrt{F} \right)^{-2} \right\}. \end{aligned} \quad (46)$$

4.2 Expectation values for $\langle T \rangle$ and $\langle \hat{P}^2 \rangle$

Substituting $q = \mu$ into Eq. (38), we have

$$\frac{\partial E_{nl}(\mu)}{\partial \mu} = \langle \psi_{nl}(\mu) \left| \frac{\partial \hat{H}(\mu)}{\partial \mu} \right| \psi_{nl}(\mu) \rangle. \quad (47)$$

Partial derivative of Eq. (39) with respect to μ gives

$$\frac{\partial H(\mu)}{\partial \mu} = -\frac{1}{\mu} \left(-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} - \frac{\hbar^2}{2\mu r} \frac{d}{dr} + \frac{\hbar^2}{2\mu r^2} l(l+1) \right). \quad (48)$$

Equation (48) implies

$$-\frac{1}{\mu}\langle T \rangle = -\frac{1}{\mu}(H - V). \quad (49)$$

Hence,

$$\langle \psi_{nl}(\mu) \left| \frac{\partial \hat{H}(\mu)}{\partial \mu} \right| \psi_{nl}(\mu) \rangle = -\frac{1}{\mu}\langle T \rangle. \quad (50)$$

From the relation $T = p^2/2\mu$, substituting for T in Eq. (49), we have

$$-\frac{1}{\mu}\langle T \rangle = -\frac{1}{2\mu^2}\langle \hat{P}^2 \rangle. \quad (51)$$

Plugging Eq. (51) into Eq. (50) yields

$$\langle \psi_{nl}(\mu) \left| \frac{\partial \hat{H}(\mu)}{\partial \mu} \right| \psi_{nl}(\mu) \rangle = -\frac{1}{2\mu^2}\langle \hat{P}^2 \rangle. \quad (52)$$

Partial derivative of Eq. (27) with respect to μ gives

$$\begin{aligned} \frac{\partial E_{nl}(\mu)}{\partial \mu} = & -\frac{\vartheta \hbar^2 l(l+1)}{2\mu^2} + 2BV \left\{ \frac{D_e r_e^2}{\hbar^2 \sqrt{F}} - \left[\left(n + \frac{1}{2} + \sqrt{F} \left(\frac{2V_0}{\vartheta^2 \hbar^2} + \frac{4D_e r_e}{\hbar^2 \vartheta} \right) \right) \right. \right. \\ & \left. \left. - \left(\frac{2Z_1}{\vartheta^2 \hbar^2} + \frac{4D_e r_e}{\hbar^2 \vartheta} + l(l+1) \right) \frac{D_e r_e^2}{\hbar^2 \sqrt{F}} \right] \left(n + \frac{1}{2} + \sqrt{F} \right)^{-2} \right\}. \quad (53) \end{aligned}$$

Connecting Eqs. (50) and (53) yields the expectation values of $\langle T \rangle$. Hence,

$$\begin{aligned} \langle T \rangle = & \frac{\vartheta \hbar^2 l(l+1)}{2\mu} - \frac{\hbar^2 \vartheta^2 \mu}{4\mu^2} V \left\{ \frac{D_e r_e^2}{\hbar^2 \sqrt{F}} - \left[\left(n + \frac{1}{2} + \sqrt{F} \left(\frac{2V_0}{\vartheta^2 \hbar^2} + \frac{4D_e r_e}{\hbar^2 \vartheta} \right) \right) \right. \right. \\ & \left. \left. - \left(\frac{2V_0}{\vartheta^2 \hbar^2} + \frac{4D_e r_e}{\hbar^2 \vartheta} + l(l+1) \right) \frac{D_e r_e^2}{\hbar^2 \sqrt{F}} \right] \left(n + \frac{1}{2} + \sqrt{F} \right)^{-2} \right\}. \quad (54) \end{aligned}$$

Connecting Eqs. (52) and (53) yields the expectation values of $\langle \hat{P}^2 \rangle$. Hence,

$$\begin{aligned} \langle \hat{P}^2 \rangle = & \vartheta \hbar^2 l(l+1) - \frac{\hbar^2 \vartheta^2}{2} V \left\{ \frac{D_e r_e^2}{\hbar^2 \sqrt{F}} - \left[\left(n + \frac{1}{2} + \sqrt{F} \left(\frac{2V_0}{\vartheta^2 \hbar^2} + \frac{4D_e r_e}{\hbar^2 \vartheta} \right) \right) \right. \right. \\ & \left. \left. - \left(\frac{2Z_1}{\vartheta^2 \hbar^2} + \frac{4D_e r_e}{\hbar^2 \vartheta} + l(l+1) \right) \frac{D_e r_e^2}{\hbar^2 \sqrt{F}} \right] \left(n + \frac{1}{2} + \sqrt{F} \right)^{-2} \right\} \quad (55) \end{aligned}$$

5 Results and Discussion

Using Eq. (27) with the spectroscopic data of Ref. [58] as presented in Table 1, also using the conversion $\hbar c = 1973.29 \text{ eV\AA}$ [59], we compute the energy spectra of the Hulthén plus screened Kratzer potential for H_2 and N_2 diatomic molecules as shown in Tables 2 and 3. It is observed that for each vibrational quantum number, the vibrational energies increase with an increase in the rotational quantum number, for each of the diatomic molecules. In addition, the energy equation of the Hulthén plus screened Kratzer potential was employed

Table 1. Parameters of selected DMs used in this study [58]

Molecules	D_e (eV)	α (\AA^{-1})	r_e (\AA)	μ (MeV)
N_2	11.93819	2.6986	1.0940	0.65235787010
H_2	4.744600	1.9426	0.7416	0.05021684305

Table 2. Energy spectra E_{nl} and expectation values for $\langle r^{-2} \rangle_{nl}$, $\langle T \rangle_{nl}$ and $\langle P^2 \rangle_{nl}$ of the HSKP for H_2 molecules

n	l	E_{nl} (eV)	$\langle r^{-2} \rangle_{nl}$ (\AA^{-2})	$\langle T \rangle_{nl}$ (eV)	$\langle P^2 \rangle_{nl}$ (eV/c) ²
0	0	-0.651520223	1.4461305900	-1.527357607	-0.2430954250
1	0	-0.694545926	0.4934942126	-1.527879485	-0.2365343415
	1	-0.837306330	0.3089006158	-1.528850921	-0.2230060212
2	0	-0.768651215	0.2328634781	-1.530131019	-0.2018428796
	1	-0.937373235	0.1919356503	-1.531517495	-0.1723326932
	2	-1.209312076	0.1661204903	-1.532756774	-0.1339118832
3	0	-0.872713066	1.5187697310	-1.512273934	-0.2397598466
	1	-1.069404202	0.5157465898	-1.512585935	-0.2328013301
	2	-1.365597788	0.3200992442	-1.513146168	-0.2185951989
	3	-1.767342813	0.2388704404	-1.513830364	-0.1966640774
4	0	-1.006593123	0.1949209917	-1.514459993	-0.1664947819
	1	-1.232063881	0.1672300249	-1.514811074	-0.1276768573
	2	-1.554585330	1.5676664310	-1.499019961	-0.2380244021
	3	-1.979646890	0.5306022009	-1.499146722	-0.2307718818
	4	-2.511388384	0.3274233022	-1.499343883	-0.2160599846
5	0	-1.170257245	0.2426244599	-1.499501576	-0.1935463559
	1	-1.424894724	0.1965821729	-1.499461878	-0.1628618456
	2	-1.774901763	0.1675873809	-1.499026507	-0.1237106879
	3	-2.225143077	1.6000110030	-1.487438213	-0.2375700761
	4	-2.779627564	0.5402950041	-1.487400766	-0.2300928725
	5	-2.779627564	0.3320371224	-1.487275955	-0.2149910763

Table 3. Energy spectra E_{nl} and expectation values for $\langle r^{-2} \rangle_{nl}$, $\langle T \rangle_{nl}$ and $\langle P^2 \rangle_{nl}$ of the HSKP for N_2 molecules

n	l	E_{nl} (eV)	$\langle r^{-2} \rangle_{nl}$ (\AA^{-2})	$\langle T \rangle_{nl}$ (eV)	$\langle P^2 \rangle_{nl}$ (eV/c) ²
0	0	-2.740002210	0.48384419100	-1.529859845	-2.733360767
1	0	-2.237811440	0.16604146380	-1.531954979	-2.742387859
	1	-2.166221765	0.10527772010	-1.536098894	-2.751403066
2	0	-2.149557432	0.08115099160	-1.542199980	-2.764720459
	1	-2.135514463	0.06914333150	-1.550123565	-2.782099026
	2	-2.145938459	0.06254753050	-1.559695049	-2.803226301
3	0	-2.124272714	0.60792631400	-1.518791268	-2.718030441
	1	-2.127449959	0.20701468020	-1.520693254	-2.722233863
	2	-2.145041222	0.12940273500	-1.524454369	-2.730564012
	3	-2.173027661	0.09790208600	-1.529989917	-2.742869320
4	0	-2.118718092	0.08168807260	-1.537175349	-2.758926885
	1	-2.129592631	0.07233546910	-1.545849125	-2.778447621
	2	-2.151297128	0.71587103800	-1.508675050	-2.699926444
	3	-2.182002364	0.24265837200	-1.510399495	-2.703812140
5	4	-2.221075461	0.15038870280	-1.513808697	-2.711512506
	0	-2.122224156	0.11247235160	-1.518824211	-2.722887159
	1	-2.740002210	0.09259811150	-1.525330645	-2.737729591
	2	-2.237811440	0.08084615000	-1.525330645	-2.755771878
	3	-2.166221765	0.81001512100	-1.499451470	-2.683419916
	4	-2.149557432	0.27374373700	-1.501012381	-2.687012953
	5	-2.135514463	0.16868922100	-1.504097390	-2.694133144

to study the expectation values of $\langle r^{-2} \rangle$, $\langle T \rangle$ and $\langle \hat{P}^2 \rangle$ for selected diatomic molecules and the numerical computations are presented in Tables 2 and 3. The results show that as the vibrational quantum number increases, the expectation values of $\langle r^{-2} \rangle$ decreases. The expectation values of $\langle T \rangle$ and $\langle \hat{P}^2 \rangle$ were obtain and seen to increase with an increase in the rotational quantum number, for the selected diatomic molecules. In Table 4, we presented energy eigenvalues of Hulthén potential. As the screening parameter increases, the energy eigenvalues increase with an increase in the quantum numbers which agrees with the reports of others.

In Figure 1 (a) and (b), the energy eigenvalues of the Hulthén plus screened Kratzer potential for ground state $n = 0$ and first excited state $n = 1$ are plotted, for different l . From the plot, the energy eigenvalue decreases, i.e., more attractive with an increase in orbital quantum number l .

Table 4. Bound states energy eigenvalues of the HP ($\hbar = \mu = 1$)

State	ϑ	Present (NUFA)	AIM [21]	EQR [11]	SUSY [23]
2p	0.025	-0.11281250000	-0.1128125	-0.1128125	-0.1127605
	0.050	-0.10125000000	-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

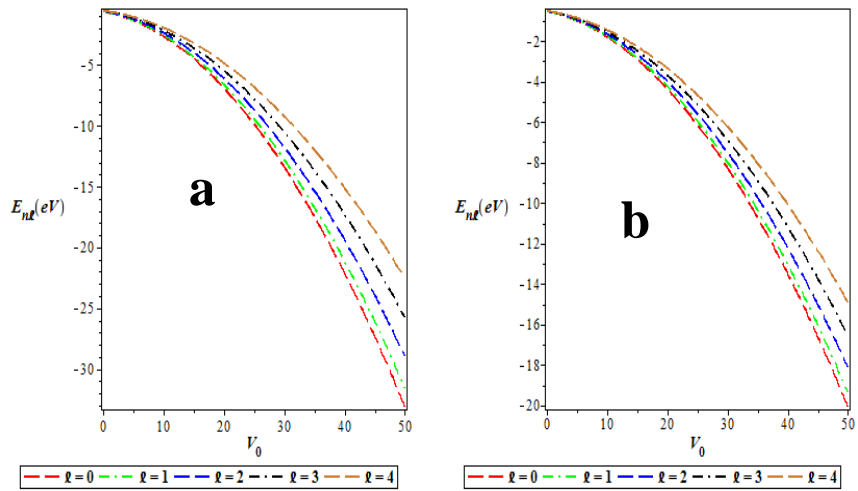


Figure 1. (a) The plot of ground state energy spectra for various l as a function of V_0 . (b) The plot of the first excited state energy spectra for different l as a function of V_0 .

6 Conclusion

In this research, the solution of the Schrodinger equation with the Hulthén plus screened Kratzer potential have been obtained within the Greene-Aldrich approximation scheme using the Nikiforov–Uvarov Functional Analysis (NUFA) method. We then apply the energy equation to study the energy spectra and the expectation values $\langle r^{-2} \rangle$, $\langle T \rangle$ and $\langle \hat{P}^2 \rangle$ using Hellmann–Feynman theorem of the Hydrogen (H_2) and Nitrogen (N_2) diatomic molecules. The results show that the bound state energy spectra of these molecules increase as various quantum numbers n and l increase. We also computed the bound state energy of Hulthén potential and our results are consistent with reported results in existing literature. The special case energy equations obtained from the NUFA method were the same when compared to other analytical methods, and this validate a high level of mathematical precision of our method.

Declarations

Availability of data and materials: All data generated during this study are included in the references in the paper.

Competing interests: The authors declare that they have no competing interests.

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Authors contributions: EPI suggested the research and the writing of the full manuscript. ESW obtain the numericals and analyzed the results. EO carried out graphical presentation. FA proofread and makes appropriate corrections in the manuscript. All authors read and approved the final manuscript.

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