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SOLUTIONS OF THE SCHRÖDINGER EQUATION WITH HULTHÉN-SCREENED KRATZER POTENTIAL: APPLICATION TO DIATOMIC MOLECULES[†]

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In this study, the Schrödinger equation with the Hulthén plus screened Kratzer potentials (HSKP) are solved via the Nikiforov-Uvarov (NU) and the series expansion methods. We obtained the energy equation and the wave function in closed form with Greene-Aldrich approximation via the NU method. The series expansion method was also used to obtain the energy equation of HSKP. Three distinct cases were obtained from the combined potentials. The energy eigenvalues of HSKP for HCl, LiH, H_2, and NO diatomic molecules were computed for various quantum states. To test the accuracy of our results, we computed the bound states energy of HCl and LiH, for a special case of Kratzer and screened Kratzer potentials, which are in excellent agreement with the report of other researchers.
Keywords: Schrödinger equation; Nikiforov-Uvarov method; series expansion method; Hulthén plus screened Kratzer Potentials; Diatomic molecules
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The determination of the dynamics of non-relativistic particles in quantum mechanics such as, the thermodynamic properties of the system, mass spectra of mesons, among others, is possible through the solutions of the Schrödinger equation (SE) [1-5]. The solutions of the SE with dissimilar potential functions have been investigated by many authors [6-10]. Also, different methods have been employed in obtaining either exact or approximate solutions of the SE such as, Asymptotic iteration method (AIM) [11,12], Laplace transformation method [13,14], super symmetric quantum mechanics (SUSYQM) [15], the Nikiforov-Uvarov (NU) method [16-28], the Nikiforov-Uvarov-Functional Analysis (NUFA) method [29], the series expansion method (SEM) [30-34], the analytical exact iterative method (AEIM) [35], the WKB approximation method [36-41] and others [42,43].

Recently, many authors have devoted interest in investigating bound states energy of countless diatomic molecules (DMs) with a single potential function and a combined potential function [44-46]. For instance, Inyang et al., [47] combined Eckart and Hellmann potential function to study some selected DMs. Also, Obogo et al. [48], investigated some selected DMs through the solution of SE with a combined potential using the NU method. In addition, Edet and Ikot, [49] studied some DMs with the shifted Deng-Fan potential. Furthermore, Edet et al. [50] studied some DMs with Deng-Fan plus Eckart potentials. Motivated by the success of other researchers, we seek to combine Hulthén plus screened Kratzer potentials (HSKP) to study selected DMs through the solutions of the SE using the NU and series expansion methods. The Hulthén potential (HP) [51] is vital in exploring the interaction existing between two particles. It is useful in areas of nuclear and molecular physics, atomic physics, condensed matter physics, and chemical physics [52].

On the other hand, Ikot et al. [53] proposed the screened Kratzer potential (SKP), which finds application in molecular physics, and many authors have employed in literature [54-56].

The aim of this study is to obtain the solutions to the SE with the HSKP and apply it to study some selected DMs. The essence of combining at least two potential models is to have a better results, because potential with more fitting parameters tends to give a better results [57]. The combined potential is of the form:

$$V(p)=-\frac{Z_1e^{-\vartheta p}}{1-e^{-\vartheta p}}-\frac{Z_2e^{-\vartheta p}}{p}+\frac{Z_3e^{-\vartheta p}}{p^2}, \tag{1}$$

where Z_1 is the potential strength for Hulthén, ϑ is the screening parameter. The letter $Z_2\equiv 2D_er_e$ and $Z_3\equiv D_er_e^2$, here D_e is dissociation energy and r_e is the equilibrium bond length.

THE SOLUTIONS OF THE SE WITH HSKP VIA THE NU METHOD

In this research, the NU method [58] and SEM [59] is adopted, which are based on solving the second-order differential equation. The details of the NU can be found in Ref. [58]. The SE characterized by a given potential $V(p)$ reads [60]:

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

where $\Psi_{nl}(p)$ is the Eigen functions, E_{nl} is the energy eigenvalues of the quantum system, μ is the reduced mass of the system, $\hbar$ is the reduced Planck's constant and p is radial distance from the origin.
Substituting Eq. (1) into Eq. (2) gives Eq. (3),

$$\frac{d^2\Psi_{nl}(p)}{dp^2}+\left[\frac{2\mu E_{nl}}{\hbar^2}+\frac{2\mu Z_1 e^{-\vartheta p}}{\hbar^2\left(1-e^{\vartheta p}\right)}+\frac{2\mu Z_2 e^{-\vartheta p}}{\hbar^2 p}-\frac{2\mu Z_3 e^{-\vartheta p}}{\hbar^2 p^2}-\frac{l(l+1)}{p^2}\right]\Psi_{nl}(p)=0 \tag{3}$$

To solve Eq. (3), the Greene-Aldrich approximation scheme [61] is introduce to deal with the centrifugal obstacle. This scheme is a good approximation to the centrifugal obstacle which is valid for $\vartheta<<1$, and its reads,

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

Pluging Eq. (4), to Eq. (3), Eq.(5) is

$$\frac{d^2\psi_{nl}(p)}{dp^2}+\left[\frac{2\mu E_{nl}}{\hbar^2}+\frac{2\mu Z_1 e^{-\vartheta p}}{\hbar^2\left(1-e^{-\vartheta p}\right)}+\frac{2\mu Z_2\vartheta e^{-\vartheta p}}{\hbar^2\left(1-e^{-\vartheta p}\right)}-\frac{2\mu Z_3\vartheta^2 e^{-\vartheta p}}{\hbar^2\left(1-e^{-\vartheta p}\right)^2}-\frac{\vartheta^2 l(l+1)}{\left(1-e^{-\vartheta p}\right)^2}\right]\psi_{nl}(p)=0 \tag{5}$$

We set

$$y=e^{-\vartheta p}. \tag{6}$$

Differentiating Eq. (6), we have Eq. (7) as,

$$\frac{d^2\Psi(p)}{dp^2}=\vartheta^2y^2\frac{d^2\Psi(y)}{dy^2}+\vartheta^2y\frac{d\Psi(y)}{dy} \tag{7}$$

Putting Eqs. (6) and (7) into Eq. (5) and after some simplifications, we have:

$$\frac{d^2\Psi(y)}{dy^2}+\frac{1-y}{y(1-y)}\frac{d\Psi(y)}{dy}+\frac{1}{y^2(1-y)^2}\left[-(\varepsilon+\eta_0)y^2+(2\varepsilon+\eta_0-\eta_1)y-(\varepsilon+\gamma)\right]\Psi(y)=0, \tag{8}$$

where

$$-\varepsilon=\frac{2\mu E_{nl}}{\vartheta^2\hbar^2},\quad \eta_0=\frac{2\mu Z_1}{\vartheta^2\hbar^2}+\frac{2\mu Z_2}{\vartheta\hbar^2},\quad \eta_1=\frac{2\mu Z_3}{\hbar^2},\quad \gamma=l(l+1)\Big\}. \tag{9}$$

Linking Eq. (8) and Eq. (1) of Ref. [58], we have:

$$\left.\begin{aligned}&\tilde{\tau}(y)=1-y;\ \sigma(y)=y(1-y);\ \sigma'(y)=1-2y,\ \sigma''(y)=-2;\\&\tilde{\sigma}(y)=-(\varepsilon+\eta_0)y^2+(2\varepsilon+\eta_0-\eta_1)y-(\varepsilon+\gamma)\end{aligned}\right\}. \tag{10}$$

Inserting Eq. (10) into Eq. (11) of Ref. [58], gives:

$$\pi(y)=-\frac{y}{2}\pm\sqrt{(B_1-K)y^2+(K+B_2)y+B_3}, \tag{11}$$

where

$$B_1=\left(\frac{1}{4}+\varepsilon+\eta_0\right),\ B_2=-(2\varepsilon-\eta_0-\eta_1),\ B_3=(\varepsilon+\gamma)\Big\}. \tag{12}$$

We take the discriminant of Eq. (11) under the square root sign and solve for K. Here, for bound state, the negative root is taken as:

$$K=-(B_2+2B_3)-2\sqrt{B_3}\sqrt{B_3+B_2+B_1}. \tag{13}$$

Substituting Eq. (13) into Eq. (11), Eq. (14) is gotten as,

$$\pi(y) = -\frac{y}{2} - \left[\left(\sqrt{B_3} + \sqrt{B_3 + B_2 + B_1} \right) y - \sqrt{B_3} \right], \tag{14}$$

Using Eq. (10) and Eq. (13), we obtain $\tau(y)$ and $\tau'(y)$ as follows:

$$\tau(y) = 1 - 2y - 2\sqrt{B_3}\, y - 2\sqrt{B_3 + B_2 + B_1}\, y + 2\sqrt{B_3}, \tag{15}$$

$$\tau'(y) = -2\left[1 + \sqrt{B_3} + \sqrt{B_3 + B_2 + B_1} \right], \tag{16}$$

where $\tau'(y)$ is the first derivative of $\tau(y)$. Referring to Eq. (10) and Eq. (13) of Ref. [58], the following equations for λ_n and λ are as follows:

$$\lambda_n = n^2 + \left[1 + 2\sqrt{B_3} + 2\sqrt{B_3 + B_2 + B_1} \right] n, \ (n = 0,1,2,...), \tag{17}$$

$$\lambda = -\frac{1}{2} - \sqrt{B_3} - \sqrt{B_3 + B_2 + B_1} - (B_2 + 2B_3) - 2\sqrt{B_3}\sqrt{B_3 + B_2 + B_1}, \tag{18}$$

When linking Eqs. (17) and (18) with the help of Eq. (9), we obtain the energy equation for the HSKP as:

$$E_{nl} = \frac{\vartheta^2\hbar^2 l(l+1)}{2\mu} - \frac{\vartheta^2\hbar^2}{8\mu}\left[\frac{\left(n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2} \right)^2 + \frac{2\mu D_e r_e^2}{\hbar^2}} \right)^2 - \frac{2\mu Z_1}{\vartheta^2\hbar^2} + \frac{4\mu D_e r_e}{\hbar^2\vartheta} + l(l+1)}{n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2} \right)^2 + \frac{2\mu D_e r_e^2}{\hbar^2}}} \right]^2. \tag{19}$$

The wave function $\phi(y)$ and weight function $\rho(y)$ is obtain by inserting the values of $\sigma(y)$, $\pi(y)$, and $\tau(y)$ given in Eqs. (10), (14) and (15), respectively, into Eq. (3) and Eq. (9) of Ref. [58] as follows:

$$\phi(y) = y^{\sqrt{B_3}} (1-y)^{\left(\frac{1}{2} + \sqrt{B_3 + B_2 + B_1} \right)}, \tag{20}$$

$$\rho(y) = y^{2\sqrt{B_3}} (1-y)^{2\sqrt{B_3 + B_2 + B_1}}. \tag{21}$$

Putting Eqs. (10) and (21), into Eq. (2) of Ref. [66], the Rodrigues relation is written as

$$y_n = B_n y^{-2\sqrt{B_3}} (1-y)^{-2\sqrt{B_3 + B_2 + B_1}} \frac{d^n}{dy^n}\left[y^{n+2\sqrt{B_3}} (1-y)^{n+2\sqrt{B_3 + B_2 + B_1}} \right], \tag{22}$$

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

$$\psi_{nl}(y) = \mathrm{N}_{nl}\, y^{\sqrt{B_3}} (1-y)^{\left(\frac{1}{2} + \sqrt{B_3 + B_2 + B_1} \right)} P_n^{\left(2\sqrt{B_3}, 2\sqrt{B_3 + B_2 + B_1} \right)} (1-2y), \tag{23}$$

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

$$\frac{\mathrm{N}_{nl}^2}{\vartheta}\int_{-1}^{1} \left(\frac{1-y}{2} \right)^{2\sqrt{B_3}} \left(\frac{1+x}{2} \right)^{\varpi} \left[A_n^{\left(2\sqrt{B_3}, 2\varpi - 1 \right)}(x) \right]^2 dx = 1, \tag{24}$$

where

$$\left.\begin{aligned} \mathrm{X} &= 1 + 2\sqrt{B_3 + B_2 + B_1}, \\ \mathrm{X} - 1 &= 2\sqrt{B_3 + B_2 + B_1} \end{aligned}\right\}. \tag{25}$$

Linking Eq. (26) with the usual integral of the form of Eq. (37) of Ref. [71],

$$\int_{-1}^{1} \left(\frac{1-A}{2} \right)^u \left(\frac{1+x}{2} \right)^v \left(A_n^{(2u, 2v-1)}(a) \right)^2 dp = \frac{2\Gamma(u+n+1)\Gamma(v+n+1)}{n!u\Gamma(u+v+n+1)}. \tag{26}$$

Hereafter, the normalization constant is

$$\mathrm{N}_{nl}=\left[\frac{n!2\sqrt{B_3}\ \vartheta\,\Gamma\left(2\sqrt{B_3}+2\sqrt{B_3+B_2+B_1}+n+2\right)}{2\Gamma\left(2\sqrt{B_3}+n+1\right)\Gamma\left(2\sqrt{B_3+B_2+B_1}+n+2\right)}\right]^{\frac{1}{2}}. \tag{27}$$

THE SOLUTIONS OF THE SE WITH THE HSKP VIA THE SEM

In order to solve the SE with SEM. The SE of the form is considered [30],

$$\frac{d^2U(p)}{dp^2}+\frac{2}{p}\frac{dU(p)}{dp}+\left[\frac{2\mu}{\hbar^2}\left(E_{nl}-V(p)\right)-\frac{l(l+1)}{p^2}\right]U(p)=0 \tag{28}$$

where l is angular quantum number, μ is the reduced mass, p is the inter-nuclear separation and E_{nl} is the energy eigenvalues.

Next, the Tylor series of the exponential terms in Eq. (1) up to order three is carried out, and then substitute back into Eq.(1), yields:

$$V(p)=-\frac{H_0}{p}+H_1p+H_2p^2+\frac{H_3}{p^2}+H_4 \tag{29}$$

where

$$\left.\begin{aligned}H_0&=-\frac{Z_1}{\vartheta}-Z_2-\vartheta Z_3,\ \mathrm{H}_1=-\frac{Z_1\vartheta}{12}-\frac{\vartheta^2Z_2}{2}-1.33Z_3\vartheta^2\\ H_2&=\frac{Z_2\vartheta^3}{6},\ \mathrm{H}_3=Z_3,\ \mathrm{H}_4=\frac{Z_1}{2}+Z_2\vartheta+Z_3\vartheta^2\end{aligned}\right\}. \tag{30}$$

By putting Eq. (29) into Eq. (28), we have,

$$\frac{d^2U(p)}{dp^2}+\frac{2}{p}\frac{dU(p)}{dp}+\left[\varepsilon+\frac{\kappa_1}{p}-\kappa_2p-\kappa_3p^2-\frac{T(T+1)}{p^2}\right]U(p)=0, \tag{31}$$

where

$$\left.\begin{aligned}\varepsilon&=\frac{2\mu}{\hbar^2}\left(E_{nl}-H_4\right),\ \kappa_1=\frac{2\mu H_0}{\hbar^2}\\ \kappa_2&=\frac{2\mu H_1}{\hbar^2},\ \kappa_3=\frac{2\mu H_2}{\hbar^2}\end{aligned}\right\}, \tag{32}$$

$$T\left(T+1\right)=\frac{2\mu H_3}{\hbar^2}+l\left(l+1\right). \tag{33}$$

From Eq. (33), we have

$$T=-\frac{1}{2}+\frac{1}{2}\sqrt{\left(2l+1\right)^2+\frac{8\mu H_3}{\hbar^2}} \tag{34}$$

The ansatz wave function is of the form [59],

$$U(p)=e^{-\sigma p^2-\rho p}S(p), \tag{35}$$

where σ and ρ are constant.

Differentiating Eq. (35), Eqs. (36) and (37) are obtain,

$$U'(p)=S'(p)\mathrm{e}^{-\sigma p^2-\rho p}+S(p)\left(-2\sigma p-\rho\right)e^{-\sigma p^2-\rho p}, \tag{36}$$

$$\begin{aligned}U''(p)&=S''(p)\mathrm{e}^{-\sigma p^2-\rho p}+S'(p)\left(-2\sigma p-\rho\right)e^{-\sigma p^2-\rho p}\\ &+\left[\left(-2\sigma\right)+\left(-2\sigma p-\rho\right)\left(-2\sigma p-\rho\right)\right]S(p)e^{-\sigma p^2-\rho p}\end{aligned}. \tag{37}$$

Upon the substitution of Eqs. (35), (36) and (37) into Eq. (31) and subsequent division by $e^{-\sigma p^2-\rho p}$, Eq. (38) is obtained:

$$S''(p)+\left[-4\sigma p-2\rho+\frac{2}{p}\right]S'(p)+\left[\begin{array}{l}\left(4\sigma^2-\kappa_3\right)p^2+\left(4\sigma\rho-\kappa_2\right)p\\+\left(\kappa_1-2\rho\right)\frac{1}{p}-\frac{T(T+1)}{p^2}+\left(\varepsilon+\rho^2-6\sigma\right)\end{array}\right]S(p)=0. \tag{38}$$

The function $S(p)$ is considered as a series of the form [59]

$$S(p)=\sum_{n=0}^{\infty}a_n p^{2n+T}. \tag{39}$$

Taking the first and second derivatives of Eq. (39) gives,

$$S'(p)=\sum_{n=0}^{\infty}(2n+T)a_n p^{2n+T-1}. \tag{40}$$

$$S''(p)=\sum_{n=0}^{\infty}(2n+T)(2n+T-1)a_n p^{2n+T-2}. \tag{41}$$

Substituting Eqs. (39), (40) and (41) into Eq. (38), we get

$$\begin{array}{l}\sum_{n=0}^{\infty}(2n+T)(2n+T-1)a_n p^{2n+T-2}+\left[-4\sigma p-2\rho+\frac{2}{p}\right]\sum_{n=0}^{\infty}(2n+T)a_n p^{2n+T-1}\\+\left[\left(4\sigma^2-\kappa_3\right)p^2+\left(4\sigma\rho-\kappa_2\right)p+\frac{\left(\kappa_1-2\rho\right)}{p}-\frac{T(T+1)}{p^2}+\left(\varepsilon+\rho^2-6\sigma\right)\right]\sum_{n=0}^{\infty}a_n p^{2n+T}=0\end{array}. \tag{42}$$

Collecting powers of p in Eq. (42) gives,

$$\sum_{n=0}^{\infty}a_n\left\{\begin{array}{l}\left[(2n+T)(2n+T-1)+2(2n+T)-T(T+1)\right]p^{2n+T-2}\\+\left[-2\rho(2n+T)+\left(\kappa_1-2\rho\right)\right]p^{2n+T-1}\\+\left[-4\sigma(2n+T)+\varepsilon+\rho^2-6\sigma\right]p^{2n+T}\\+\left[4\alpha\beta-\xi_2\right]r^{2n+L+1}+\left[4\alpha^2-\xi_3\right]r^{2n+L+2}\end{array}\right\}=0. \tag{43}$$

Equation (43) is linearly independent, noting that p is a non-zero function; consequently, it is the coefficient of P that is zero. With this, we have,

$$(2n+T)(2n+T-1)+2(2n+T)-T(T+1)=0, \tag{44}$$

$$-2\rho(2n+T)+\kappa_1-2\rho=0, \tag{45}$$

$$-4\sigma(2n+T)+\varepsilon+\rho^2-6\sigma=0, \tag{46}$$

$$4\sigma\rho-\kappa_2=0, \tag{47}$$

$$4\sigma^2-\kappa_3=0. \tag{48}$$

From Eqs. (45) and (48) we have

$$\rho=\frac{\kappa_1}{2(2n+T+1)}. \tag{49}$$

$$\sigma=\frac{\sqrt{\kappa_3}}{2}. \tag{50}$$

We proceed to obtaining the energy equation using Eq. (46) and have

$$\varepsilon=2\sigma(4n+2T+3)-\rho^2. \tag{51}$$

By substituting Eqs. (32), (34), (49) and (34) into Eq. (51) and simplifying we obtain

$$E_{nl}=\sqrt{\frac{\hbar^2 H_2}{2\mu}}\left(4n+2+\sqrt{(2l+1)^2+\frac{8\mu H_3}{\hbar^2}}\right)-\frac{2\mu H_0^2}{\hbar^2}\left(4n+1+\sqrt{(2l+1)^2+\frac{8\mu H_3}{\hbar^2}}\right)^{-2}+H_4. \tag{52}$$

Upon substituting Eq. (30) into Eq. (52) we obtain the energy eigenvalues of the HSKP as,

$$\begin{aligned}E_{nl}=&\sqrt{\frac{\hbar^2 D_e r_e \vartheta^3}{6\mu}}\left(4n+2+\sqrt{(2l+1)^2+\frac{8\mu D_e r_e^2}{\hbar^2}}\right)\\&-\frac{2\mu}{\hbar^2}\left(-\frac{Z_1}{\vartheta}-2D_e r_e-\vartheta D_e r_e^2\right)^2\left(4n+1+\sqrt{(2l+1)^2+\frac{8\mu D_e r_e^2}{\hbar^2}}\right)^{-2}+\frac{Z_1}{2}+2D_e r_e\vartheta+D_e r_e^2\vartheta^2\end{aligned}. \tag{53}$$

Special cases of the HSKP

1. In the case $Z_2=Z_3=0$ we have the HP of Eq. (54) and its energy equation of Eq. (55)

$$V(p)=-\frac{Z_1 e^{-\vartheta p}}{1-e^{-\vartheta p}}, \tag{54}$$

$$E_{nl}=\frac{\vartheta^2\hbar^2 l(l+1)}{2\mu}-\frac{\vartheta^2\hbar^2}{8\mu}\left[\frac{(n+l+1)^2-\frac{2\mu Z_1}{\vartheta^2\hbar^2}+l(l+1)}{n+l+1}\right]^2. \tag{55}$$

Equation (55) is in agreement with Eq. (32) of [8] and Eq. (37) of [6].

2. By setting $Z_1=0$ we have the SKP of Eq. (56) and its energy equation of Eq. (57)

$$V(p)=-\frac{Z_2 e^{-\vartheta p}}{p}+\frac{Z_3 e^{-\vartheta p}}{p^2}, \tag{56}$$

$$E_{nl}=\frac{\vartheta^2\hbar^2 l(l+1)}{2\mu}-\frac{\vartheta^2\hbar^2}{8\mu}\left[\frac{\left(n+\frac{1}{2}+\sqrt{\left(l+\frac{1}{2}\right)^2+\frac{2\mu D_e r_e^2}{\hbar^2}}\right)^2+\frac{4\mu D_e r_e}{\hbar^2\vartheta}+l(l+1)}{n+\frac{1}{2}+\sqrt{\left(l+\frac{1}{2}\right)^2+\frac{2\mu D_e r_e^2}{\hbar^2}}}\right]^2. \tag{57}$$

Equation (57) agrees with Eq. (29) of [53].

3. By setting $Z_1=\vartheta=0$ we have the Kratzer potential (KP) of Eq.(58) and its energy equation of Eq. (59)

$$V(p)=-\frac{Z_2}{p}+\frac{Z_3}{p^2}, \tag{58}$$

$$E_{nl}=-\frac{2\mu D_e^2 r_e^2}{\hbar^2\left(n+\frac{1}{2}+\sqrt{\left(l+\frac{1}{2}\right)^2+\frac{2\mu D_e r_e^2}{\hbar^2}}\right)^2}. \tag{59}$$

Equation (59) agrees with Eq. (46) of [53];

RESULTS AND DISCUSSION

In the present study, we use Eqs. (19) and (53) to study the energy spectra of four selected diatomic molecules. The spectroscopic parameters of these molecules are given in Table 1 and taken from [62]. We used the following conversions factors: $\hbar c=1973.29$ eV $\mathring{A}$ and 1amu $931.5\times10^6 eV(\mathring{A})^{-1}$ for all computations [62]. The numerical computation of the energy eigenvalues of the HSKP for HCl, LiH, H_2 and NO DMs are given in Tables 2 and 3. It is observed that for each vibrational quantum number, the energy increase with increase in the rotational quantum number, for each of the selected DMs. To validate our results, we deduce Kratzer and screened Kratzer potentials from the proposed potential to compute the energy spectra for HCl and LiH DMs. It is seen that our results are in excellent agreement with the report of

Ref. [30] and Ref. [53] as shown in Tables 4 and 5. We plotted the energy eigenvalues of HSKP for selected molecules with different rotational quantum number (RQN). The plot of the energy eigenvalues of HCl and NO with different values of l is shown in Fig. 1 and Fig. 2. It depicts a monotonic decrease as the principal quantum number increases and all converges together.

Table 1. Spectroscopic parameters of selected DMs [62]

Molecules	$D_e(eV)$	$\alpha = \vartheta\left(\overset{\circ}{A}^{-1}\right)$	$r_e(\dot{A})$	$\mu(MeV)$
HCl	4.6190309050	1.86770	1.2746	0.09129614886
LiH	2.5152672118	1.12800	1.5956	0.08198284801
H_2	4.7446000000	1.94260	0.7416	0.05021684305
NO	8.0437300000	1.86430	1.1508	5.91053826200

Table 2. Bound state energy spectra $E_{nl}(eV)$ of HSKP for HCl, LiH, H_2 and NO DMs with the NU method

n	l	$E_{nl}(\text{eV})$ of HCl	$E_{nl}(\text{eV})$ of LiH	$E_{nl}(\text{eV})$ of H_2	$E_{nl}(\text{eV})$ of NO
0	0	-22.17032494	-9.044861721	-13.92974441	-34.53518839
0	1	-22.17022128	-9.044847651	-13.93464244	-34.53518812
0	2	-22.17001432	-9.044819582	-13.94456401	-34.53518756
0	3	-22.16970474	-9.044777634	-13.94456401	-34.53518674
0	4	-22.16929354	-9.044722014	-13.98060726	-34.53518565
0	5	-22.16878209	-9.044652964	-13.98060745	-34.53518429
1	0	-22.24690799	-9.033844252	-13.79739618	-34.53969898
1	1	-22.24679078	-9.033836790	-13.80084636	-34.53969869
1	2	-22.24655670	-9.033821914	-13.80786295	-34.53969812
1	3	-22.24620649	-9.033799708	-13.81867833	-34.53969726
1	4	-22.24574126	-9.033770284	-13.83364106	-34.53969611
1	5	-22.24516244	-9.033733821	-13.85321597	-34.53969468
2	0	-22.33432382	-9.029306244	-13.70661022	-34.54441426
2	1	-22.33419477	-9.029304880	-13.70872277	-34.54441398
2	2	-22.33393705	-9.029302176	-13.71305549	-34.54441337
2	3	-22.33355145	-9.029298171	-13.71982357	-34.54441248
2	4	-22.33303911	-9.029292928	-13.72934979	-34.54441128
2	5	-22.33240157	-9.029286529	-13.74206457	-34.54440980
3	0	-22.43212310	-9.030892408	-13.65662021	-34.54933324
3	1	-22.43198398	-9.030896786	-13.65749846	-34.5433292
3	2	-22.43198398	-9.030905540	-13.65935463	-34.54933232
3	3	-22.43129039	-9.030918685	-13.66238806	-34.54933137
3	4	-22.43073793	-9.030936216	-13.66689774	-34.54933014
3	5	-22.43005037	-9.030958150	-13.67328236	-34.54932858
4	0	-22.53989148	-9.038278642	-13.64667365	-34.54932858
4	1	-22.53974404	-9.038288540	-13.64641418	-34.55445454
4	2	-22.53944960	-9.038308324	-13.64598762	-34.55445388
4	3	-22.53900894	-9.038337960	-13.64557866	-34.55445292
4	4	-22.53842333	-9.038377402	-13.64546438	-34.5544162
4	5	-22.53769441	-9.038426596	-13.64601419	-34.55445003

Table 3. Bound state energy spectra $E_{nl}(eV)$ of HSKP for HCl, LiH LiH, H_2 and NO DMs with the S,EM

n	l	$E_{nl}(\text{eV})$ of HCl	$E_{nl}(\text{eV})$ of LiH	$E_{nl}(\text{eV})$ of H_2	$E_{nl}(\text{eV})$ of NO
0	0	-22.17032454	-9.044861731	-13.92974451	-34.53518830
0	1	-22.17022118	-9.044847641	-13.93464234	-34.53518813
0	2	-22.17001422	-9.044819562	-13.94456411	-34.53518757
0	3	-22.16970464	-9.044777654	-13.94456411	-34.53518674
0	4	-22.16929344	-9.044722034	-13.98060736	-34.53518566
0	5	-22.16878219	-9.044652954	-13.98060725	-34.53518420
1	0	-22.24690789	-9.033844242	-13.79739638	-34.53969899
1	1	-22.24679018	-9.033836760	-13.80084646	-34.53969865
1	2	-22.24655660	-9.033821954	-13.80786285	-34.53969813
1	3	-22.24620659	-9.033799718	-13.81867843	-34.53969726
1	4	-22.24574136	-9.033770264	-13.83364116	-34.53969612
1	5	-22.24516234	-9.033733831	-13.85321587	-34.53969469
2	0	-22.33432372	-9.029306254	-13.70661032	-34.54441427
2	1	-22.33419467	-9.029304830	-13.70872287	-34.54441399
2	2	-22.33393704	-9.029302156	-13.71305559	-34.54441338
2	3	-22.33355135	-9.029298181	-13.71982367	-34.54441249

n	l	$E_{nl}(\text{eV})$ of HCl	$E_{nl}(\text{eV})$ of LiH	$E_{nl}(\text{eV})$ of H_2	$E_{nl}(\text{eV})$ of NO
2	4	-22.33303921	-9.029292928	-13.72934989	-34.54441129
2	5	-22.33240117	-9.029286539	-13.74206467	-34.54440981
3	0	-22.43212300	-9.030892418	-13.65662031	-34.54933325
3	1	-22.43198318	-9.030896796	-13.65749856	-34.54332920
3	2	-22.43198328	-9.030905550	-13.65935443	-34.54933233
3	3	-22.43129039	-9.030918675	-13.66238816	-34.54933138
3	4	-22.43073743	-9.030936226	-13.66689784	-34.54933015
3	5	-22.43005027	-9.030958110	-13.67328246	-34.54932859
4	0	-22.53989138	-9.038278642	-13.64667375	-34.54932859
4	1	-22.53974414	-9.038288550	-13.64641428	-34.55445455
4	2	-22.53944950	-9.038308344	-13.64598772	-34.55445389
4	3	-22.53900884	-9.038337930	-13.64557886	-34.55445293
4	4	-22.53842323	-9.038377412	-13.64546408	-34.55441620
4	5	-22.53769451	-9.038426586	-13.64601429	-34.55445000

Table 4. Assessment of the Energy eigenvalues $E_{nl}(eV)$ of the KP for HCl and LiH

n	l	Present work for energy (eV) of HCl	Energy (eV) of HCl Ref. [38]	Energy (eV) of HCl Ref. [60]	Present work for energy (eV) of LiH	Energy (eV) of LiH Ref. [38]	Energy (eV) of LiH Ref. [60]
0	0	-4.54184821	-4.574322886	-4.541847882	-2.46731030	-2.467293680	-2.467293778
1	0	-4.39372795	-4.402122552	-4.393727024	-2.37581921	-2.380989203	-2.375802636
	1	-4.39129385	-4.401308521	-4.391292904	-2.37410797	-2.380416619	-2.374091378
2	0	-4.25273711	-4.239466022	-4.252735636	-2.28932426	-2.281213703	-2.289307674
	1	-4.25041920	-4.238696688	-4.250417718	-2.28770560	-2.280676728	-2.287688996
	2	-4.24579105	-4.237158875	-4.245789526	-2.28447521	-2.279603547	-2.284458584
3	0	-4.11842537	-4.085660853	-4.118423404	-2.20746820	-2.187580925	-2.207451626
	1	-4.11621638	-4.084933001	-4.116214408	-2.20593555	-2.187076666	-2.205918968
	2	-4.11180563	-4.083478096	-4.111803616	-2.20287674	-2.186068862	-2.202860140
	3	-4.10520744	-4.081297704	-4.105205380	-2.19830467	-2.184558925	-2.198288040
4	0	-3.99037742	-3.940076275	-3.990375014	-2.12992512	-2.099596786	-2.129908602
	1	-3.98827064	-3.939386976	-3.988268222	-2.12847251	-2.099122640	-2.128455976
	2	-3.98406387	-3.938009125	-3.984061424	-2.12557335	-2.098175007	-2.125556792
	3	-3.97777065	-3.935944185	-3.977768152	-2.12123970	-2.096755197	-2.121223116
	4	-3.96941113	-3.933194375	-3.969408570	-2.11548950	-2.094865172	-2.115472884
5	0	-3.86820974	-3.802136724	-3.868206938	-2.05639728	-2.016815899	-2.056380834
	1	-3.86619896	-3.801483303	-3.866196140	-2.05501922	-2.016369515	-2.055002762
	2	-3.86218380	-3.800177161	-3.862180950	-2.05226878	-2.015477357	-2.052252304
	3	-3.85617703	-3.798219664	-3.856174134	-2.04815726	-2.014140642	-2.048140758
	4	-3.84819767	-3.795612890	-3.848194720	-2.04270146	-2.012361189	-2.042684928
	5	-3.83827087	-3.792359570	-3.838267840	-2.03592352	-2.010141421	-2.035906942

Table 5. Assessment of the Energy eigenvalues $E_{nl}(eV)$ of the SKP for HCl and LIH

n	l	Present work for energy of $E_{nl}(eV)$ LiH	Present work for energy of $E_{nl}(eV)$ HCl	Energy (eV) of LiH Ref. [60]	Energy (eV) of HCl Ref. [60]
0	0	-9.070968134	-22.19329052	-9.070968135	-22.19329052
1	0	-9.059446115	-22.26953722	-9.059446120	-22.26953722
	1	-9.047056120	-22.24266011	-9.047056120	-22.24266011
2	0	-9.054431116	-22.35663288	-9.054431115	-22.35663288
	1	-9.042278085	-22.33012521	-9.042278085	-22.33012521
	2	-9.017997940	-22.27714784	-9.017997940	-22.27714784
3	0	-9.055565865	-22.45412720	-9.055565865	-22.45412720
	1	-9.043637070	-22.42797265	-9.043637070	-22.42797265
	2	-9.019803985	-22.37569979	-9.019803985	-22.37569979
	3	-8.984115355	-22.29738072	-8.984115355	-22.29738072
4	0	-9.062524470	-22.56160484	-9.062524470	-22.56160484
	1	-9.050808170	-22.53578825	-9.050808170	-22.53578825
	2	-9.027398770	-22.48418965	-9.027398770	-22.48418965
	3	-8.992342455	-22.40687787	-8.992342455	-22.40687787
	4	-8.945707875	-22.30395550	-8.945707875	-22.30395550
5	0	-9.075009170	-22.67868230	-9.075009170	-22.67868230
	1	-9.063494530	-22.65318950	-9.063494530	-22.65318950
	2	-9.040487255	-22.60223694	-9.040487255	-22.60223694
	3	-9.006031120	-22.52589037	-9.006031120	-22.52589037
	4	-8.960191210	-22.42424781	-8.960191210	-22.42424781
	5	-8.903053285	-22.29743871	-8.903053285	-22.29743871

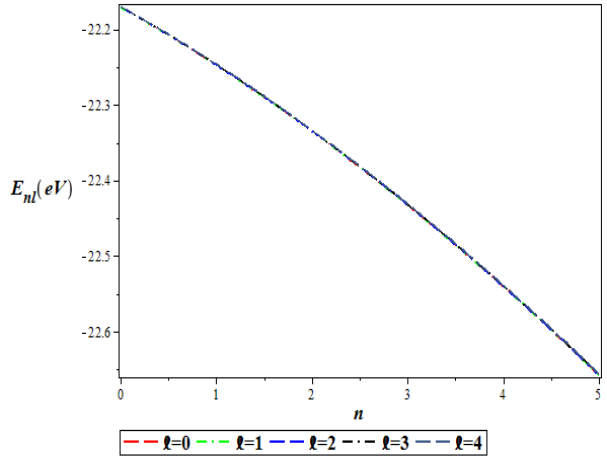

Figure 1. The plot of the energy spectra for various l versus n for HCl Diatomic molecules

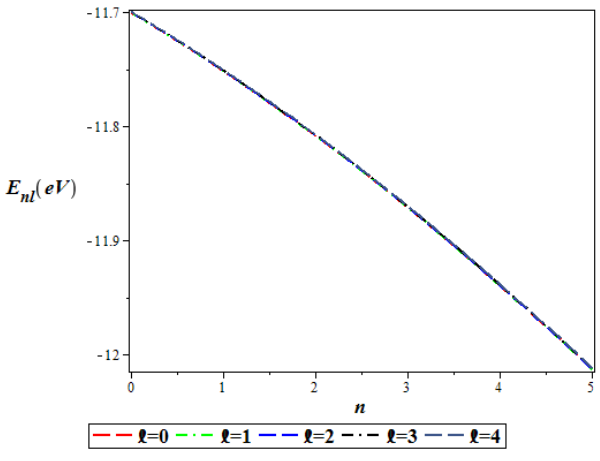

Figure 2. The plot of the energy spectra for various l versus n for NO Diatomic molecules

CONCLUSION

In this research, we solved the SE with the HSKP using the NU and series expansion methods. The energy equation and the normalized wave function were obtained. We then applied the energy equation to study four DMs. The results show that the energy spectra of these DMs increase as various quantum numbers n and l increase. To test the accuracy of our results, we computed the bound state energy of two DMs for KP and SKP, which were found to agree with the report of other researchers. Variation of the energies with respect to principal quantum number was plotted.

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РОЗВ'ЯЗАННЯ РІВНЯННЯ ШРЕДІНГЕРА З ХУЛЬТЕН-ЕКРАНОВАНИМ КРАТЦЕР ПОТЕНЦІАЛОМ: ЗАСТОСУВАННЯ ДО ДВУХАТОМНИХ МОЛЕКУЛ

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У цьому дослідженні рівняння Шредінгера з екранованими потенціалами Хультена-плюс екрановані потенціали Кратцера (HSKP) розв'язуються за допомогою методів Нікіфорова-Уварова (НУ) і розкладання в ряд. Методом NU отримано рівняння енергії та хвильова функція в закритому вигляді з наближенням Гріна-Олдріча. Метод розкладання в ряд також був використаний для отримання рівняння енергії HSKP. З об'єднаних потенціалів було отримано три різні випадки. Для різних квантових станів розраховано власні значення енергії HSKP для HCl, LiH, H_2, і NO двоатомних молекул. Щоб перевірити точність наших результатів, ми обчислили енергію зв'язаних станів HCl і LiH, для окремого випадку потенціалу Кратцера та екранованого потенціалу Кратцера, які чудово узгоджуються з результатами інших дослідників.

Ключові слова: рівняння Шредінгера; метод Нікіфорова-Уварова; метод розширення рядів; потенціал Кратцера плюс екранований Hulthén потенціал; двоатомні молекули