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Analytical solutions to the Schrödinger Equation with a Combined Potential using the Series Expansion Method to Study Selected Diatomic Molecules

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Abstract: *In this work, the Schrödinger equation with the Hulthén plus screened Kratzer Potential is solved via the series expansion method. The energy equation was used to compute the bound state energy for twelve diatomic molecules such as; CuLi, TiH, VH, TiC, HCl, LiH, H_2, ScH, CO, I_2, N_2, and NO for various quantum states. Three special cases were obtained from the combined potential when some potential parameters were set to zero, resulting in Hulthén, screened Kratzer, and Kratzer potentials. To test the accuracy of our results, we computed the bound state energy eigenvalues for HCl and LiH diatomic molecules for a special case of the Kratzer and screened Kratzer potential and the results obtained were in excellent agreement with the report of other researchers in the literature.*

Keywords: *Schrödinger equation; series expansion method; Hulthén Potential; screened Kratzer Potential; diatomic molecules*

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1.0 Introduction

The Schrodinger equation (SE) is fundamental in quantum mechanics (QM) because it defines a particle’s action in a microscopic setting. The solutions of the SE are of great importance in the determination of the dynamics of the non-relativistic particles in QM such as the thermodynamic properties of the system, and mass spectra of mesons, among others (Inyang *et al*., 2021; Allosh, *e al*., 2021; Abu-shady *et al*.,20 21;Ikot *et al*., 2020; Mutuk, 2018).

The solutions of the SE with diverse potential functions have been investigated by many authors (Horchani *et al*., 2 021;Onate *et al*., 2021; Antia *et al*. ,2015;Onate *et al*.,2018;Edit, and Okoi , 2019; Willaim *et al*., 2022; Inyang *et al*., 2021;Ita *et al*.,2018; Okon and Popoola 2015;Asp oukeh and Hamad, 2020 ;William *t al*.,2020; Prasanth *et a l*.,2020;Okorie *et al*.,2021). Also, different techniques have been employed in obtaining either exact or approximate solutions of the SE such as the asymptotic iteration method(AIM) (Rani *et a l*., 2018;Ciftci and Kisoglu,2018; Oyewumi and Oluwadare, 2016), Laplace transformation method (Abu-Shady and Khokha, 201itAbu-Shady *et al*.,2018), supersymmetric quantum mechanics (SUSYQM) (Abu-Shady and Ikot, 2019 ;Al-Jamel, 2019), the Nikiforov-Uvarov (NU) method (Ntibi *et al*.,2020 ;Okoi *et al*.,20 20;Edet *et al*.,2 019;Inyang *et al* .;021;.Edet et al.,2020; Inyang *et al*., 2020; Inyang *et al*., 2 021;Edet *et al*., 2020; Ekpo *et al*., 2020; William *et al*., 2020;Inyang *et al*.,2021; Abu-Shady *et al*., 2019;Inyang *et al*., 2021a,b,c; Omugbe, 2020; Thompson *et al*.,2022; Abu-Shady, 2016;Akpan *et al*., 2021), the Nikiforov-Uvarov Functional Analysis (NUFA) method (Ikot *et al*., 2021; Rampho *et al*.,2020, Inyang *et al*., 2022), the series expansion method (SEM) (Inyang *et al*., 2020;Ibekwe *et al*., 2020; Inyang *et al*., 2021; Abu-Shady,and Fath-Allah, 2019;Inyang *et al*.,2021;Ibekwe *et al*.,2021; Inyang *et al*., 2022), analytical exact iterative method(AEIM)(Khokha *et al*.,2016),WKB approximation method (Omugbe *et al*., 2020; Omugbe *et al*., 2021;Omugbe *et al*., 2022; Omugbe,2020 a,b;Hitler *et al*.,2017) ,Exact Quantization Rule (EQR) (Qiang *et al*., 2008;Inyang *et al*.,2020) and so on (Ali *et al*., 2020).

Recently, many authors have devoted interest in investigating the bound state energy of various diatomic molecules with a single potential function and a combined potential function (Edet *et al*., 2020; Ekwevugbe,2020; Okoi *et al*.,2020; Edet *et al*.,2020;Nwabuzor *et al*., 2021;Onate *et al*.,2021; Ikot *et al*.,2019; Horchani *et al*., 2021;Purohit *et al*., 2021). For instance, Inyang *et al*.(2021) combined Eckart and Hellmann potential functions to study some selected diatomic molecules (DMs). Also, Obogo *et al*. (2021), investigated some selected DMs through the solution of SE with q-deformed Hulthén -quadratic exponential – type potential. In addition, Edet and Ikot, (2020) studied some DMs with the shifted Deng-Fan potential. Furthermore, Edet *et al*., (2021) studied some DMs with Deng-Fan plus Eckart potentials. Motivated by the success of other researchers, we seek to study the linear combination of Hulthén plus screened Kratzer potential (HSKP) for some selected DMs through the solutions of the SE using the SEM. The Hulthén potential (HP) is essential in exploring the interaction existing between two particles (Hulthén, 1942). It is applied in nuclear and molecular physics, atomic physics, condensed matter physics, and chemical physics (Okon *et al*., 2021). The screened Kratzer potential (SKP) which was proposed by Ikot, *et al*. (2019) recently, finds application in molecular physics, and many authors have employed it in literature (Ikot *et al*., *2020a,b*; 2021 Edet *et al*.,2021;Ikot *et al*., 2021).

This study aims to obtain the approximate bound state solutions to the SE with the HSKP and apply it to study selected DMs. The essence of combining at least two potential functions is to have better results because potential with more fitting parameters tends to give a better result (Inyang et al., 2021). The combined potential reads:

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

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.

2.0 The solutions of the SE with the HSKP via the SEM

In this study, we adopt the SEM which is based on solving the second-order differential equation (Rani *et al*.,2018).

The SE of the form is considered (Rani *et al*.,2018).

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

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

The series expansion of the exponential terms in Eq. (1) up to order three is carried out and then substituted back into Eq.(1), yields,

$$V(p)=-\frac{H_0}{p}+H_1p+H_2p^2+\frac{H_3}{p^2}+H_4 \tag{3}$$

where

$$\left.\begin{aligned} &H_0=-\frac{Z_1}{\vartheta}-Z_2-\vartheta Z_3,\ \mathrm{H}_1=-\frac{Z_1\vartheta}{12}-\frac{\vartheta^2Z_2}{2}-1.33Z_3\vartheta^2 \\ &H_2=\frac{Z_2\vartheta^3}{6},\ \mathrm{H}_3=Z_3,\ \mathrm{H}_4=\frac{Z_1}{2}+Z_2\vartheta+Z_3\vartheta^2 \end{aligned}\right\} \tag{4}$$

By putting Eq. (2) into Eq. (3), we have,

$$\frac{d^2U(p)}{dp^2}+\frac{2}{p}\frac{dU(p)}{dp}+\left[\varepsilon+\frac{\kappa_1}{p}-\kappa_2p-\kappa_3p^2-\frac{T(T+1)}{p^2}\right]U(p)=0 \tag{5}$$

where

$$\left.\begin{aligned} &\varepsilon=\frac{2\mu}{\hbar^2}\left(E_{nl}-H_4\right),\ \kappa_1=\frac{2\mu H_0}{\hbar^2} \\ &\kappa_2=\frac{2\mu H_1}{\hbar^2},\ \kappa_3=\frac{2\mu H_2}{\hbar^2} \end{aligned}\right\} \tag{6}$$

$$T\left(T+1\right)=\frac{2\mu H_3}{\hbar^2}+l\left(l+1\right) \tag{7}$$

The simplification of Eq. (7),yields equation 8

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

The anzats wave function is defined as follows (Rani *et al*.,2018).

$$U(p)=e^{-\sigma p^2-\rho p}S(p) \tag{9}$$

where σ and ρ are constant.

The differentiation of Eq. (9) generates Eqs. (10) and (11) as follows:

$$U'(p)=S'(p)\mathrm{e}^{-\sigma p^2-\rho p}+S(p)\left(-2\sigma p-\rho\right)e^{-\sigma p^2-\rho p} \tag{10}$$

$$\begin{aligned} U''(p)&=S''(p)\mathrm{e}^{-\sigma p^2-\rho p}+S'(p)\left(-2\sigma p-\rho\right)e^{-\sigma p^2-\rho p} \\ &+\left[\left(-2\sigma\right)+\left(-2\sigma p-\rho\right)\left(-2\sigma p-\rho\right)\right]S(p)e^{-\sigma p^2-\rho p} \end{aligned} \tag{11}$$

Upon the substitution of Eqs. (9), (10) and, (11) into Eq. (5) and subsequent division by $e^{-\sigma p^2-\rho p}$, equation 12 is obtained:

$$S''(p)+\left[-4\sigma p-2\rho+\frac{2}{p}\right]S'(p)+\left[\begin{array}{l}\left(4\sigma^{2}-\kappa_{3}\right)p^{2}+\left(4\sigma\rho-\kappa_{2}\right)p\\ +\left(\kappa_{1}-2\rho\right)\dfrac{1}{p}-\dfrac{T(T+1)}{p^{2}}+\left(\varepsilon+\rho^{2}-6\sigma\right)\end{array}\right]S(p)=0 \tag{12}$$

The function $S(p)$ is considered as a series of the form (Rani *et al*.,2018).

$$S(p)=\sum_{n=0}^{\infty}a_{n}p^{2n+T} \tag{13}$$

The first and second derivatives of Eq. (13) gives,

$$S'(p)=\sum_{n=0}^{\infty}\left(2n+T\right)a_{n}p^{2n+T-1} \tag{14}$$

$$S''(p)=\sum_{n=0}^{\infty}\left(2n+T\right)\left(2n+T-1\right)a_{n}p^{2n+T-2} \tag{15}$$

By substituting Eqs. (13),(10)and (15) into Eq.(12) ,we get

$$\begin{array}{l}\displaystyle\sum_{n=0}^{\infty}\left(2n+T\right)\left(2n+T-1\right)a_{n}p^{2n+T-2}+\left[-4\sigma p-2\rho+\frac{2}{p}\right]\sum_{n=0}^{\infty}\left(2n+T\right)a_{n}p^{2n+T-1}\\ \displaystyle+\left[\left(4\sigma^{2}-\kappa_{3}\right)p^{2}+\left(4\sigma\rho-\kappa_{2}\right)p+\frac{\left(\kappa_{1}-2\rho\right)}{p}-\frac{T\left(T+1\right)}{p^{2}}+\left(\varepsilon+\rho^{2}-6\sigma\right)\right]\sum_{n=0}^{\infty}a_{n}p^{2n+T}=0\end{array} \tag{16}$$

Collecting powers of p in Eq. (16) gives,

$$\sum_{n=0}^{\infty}a_{n}\left\{\begin{array}{l}\left[\left(2n+T\right)\left(2n+T-1\right)+2\left(2n+T\right)-T\left(T+1\right)\right]p^{2n+T-2}\\ +\left[-2\rho\left(2n+T\right)+\left(\kappa_{1}-2\rho\right)\right]p^{2n+T-1}\\ +\left[-4\sigma\left(2n+T\right)+\varepsilon+\rho^{2}-6\sigma\right]p^{2n+T}\\ +\left[4\alpha\beta-\xi_{2}\right]p^{2n+L+1}+\left[4\alpha^{2}-\xi_{3}\right]p^{2n+L+2}\end{array}\right\}=0 \tag{17}$$

Equation (17) is linearly independent, noting that r is a non-zero function; consequently, it is the coefficient of r that is zero. With this, we have,

$$\left(2n+T\right)\left(2n+T-1\right)+2\left(2n+T\right)-T\left(T+1\right)=0 \tag{18}$$

$$-2\rho\left(2n+T\right)+\kappa_{1}-2\rho=0 \tag{19}$$

$$-4\sigma\left(2n+T\right)+\varepsilon+\rho^{2}-6\sigma=0 \tag{20}$$

$$4\sigma\rho-\kappa_{2}=0 \tag{21}$$

$$4\sigma^{2}-\kappa_{3}=0 \tag{22}$$

From Eqs. (19) and (22) we have

$$\rho=\frac{\kappa_{1}}{2(2n+T+1)} \tag{23}$$

$$\sigma=\frac{\sqrt{\kappa_{3}}}{2} \tag{24}$$

The energy equation can be obtained from equation 20 as follows:

$$\varepsilon = 2\sigma\left(4n+2T+3\right)-\rho^2 \tag{25}$$

The substitution of Eqs. (6), (8), (23) and (24) into Eq. (25) yields equation 26 upon simplification,

$$E_{nl} = \sqrt{\frac{\hbar^2 H_2}{2\mu}}\left(4n+2+\sqrt{\left(2l+1\right)^2+\frac{8\mu H_3}{\hbar^2}}\right)-\frac{2\mu H_0^2}{\hbar^2}\left(4n+1+\sqrt{\left(2l+1\right)^2+\frac{8\mu H_3}{\hbar^2}}\right)^{-2}+H_4 \tag{26}$$

Also the substitution of Eq. (4) into Eq. (26) leads to the energy eigenvalue of the HSKP as,

$$\begin{aligned} E_{nl} &= \sqrt{\frac{\hbar^2 D_e r_e \vartheta^3}{6\mu}}\left(4n+2+\sqrt{\left(2l+1\right)^2+\frac{8\mu D_e r_e^2}{\hbar^2}}\right) \\ &-\frac{2\mu}{\hbar^2}\left(-\frac{Z_1}{\vartheta}-2D_e r_e-\vartheta D_e r_e^2\right)^2\left(4n+1+\sqrt{\left(2l+1\right)^2+\frac{8\mu D_e r_e^2}{\hbar^2}}\right)^{-2}+\frac{Z_1}{2}+2D_e r_e\vartheta+D_e r_e^2\vartheta^2 \end{aligned} \tag{27}$$

Special cases of HSKP

1. In the case $Z_2 = Z_3 = 0$ we have the HP of Eq.(28) and its energy equation of Eq.(29)

$$V\left(p\right) = -\frac{Z_1 e^{-\vartheta p}}{1-e^{-\vartheta p}} \tag{28}$$

$$E_{nl} = -\frac{2\mu}{\hbar^2}\left(-\frac{Z_1}{\vartheta}\right)^2\left(4n+1+\sqrt{\left(2l+1\right)^2}\right)^{-2}+\frac{Z_1}{2} \tag{29}$$

2. By setting $Z_1 = 0$ we have the SKP of Eq.(30) and its energy equation of Eq.(31)

$$V\left(p\right) = -\frac{Z_2 e^{-\vartheta p}}{p}+\frac{Z_3 e^{-\vartheta p}}{p^2} \tag{30}$$

$$\begin{aligned} E_{nl} &= \sqrt{\frac{\hbar^2 D_e r_e \vartheta^3}{6\mu}}\left(4n+2+\sqrt{\left(2l+1\right)^2+\frac{8\mu D_e r_e^2}{\hbar^2}}\right) \\ &-\frac{2\mu}{\hbar^2}\left(-2D_e r_e-\vartheta D_e r_e^2\right)^2\left(4n+1+\sqrt{\left(2l+1\right)^2+\frac{8\mu D_e r_e^2}{\hbar^2}}\right)^{-2}+2D_e r_e\vartheta+D_e r_e^2\vartheta^2 \end{aligned} \tag{31}$$

3. By setting $Z_1 = \vartheta = 0$ we have the Kratzer potential (KP) of Eq.(32) and its energy equation of Eq. (33)

$$V\left(p\right) = -\frac{Z_2}{p}+\frac{Z_3}{p^2} \tag{32}$$

$$E_{nl} = -\frac{2\mu}{\hbar^2}\left(-2D_e r_e\right)^2\left(4n+1+\sqrt{\left(2l+1\right)^2+\frac{8\mu D_e r_e^2}{\hbar^2}}\right)^{-2} \tag{33}$$

3.0 Results and Discussion

Using Eq. (27), and the application of the spectroscopic data obtained from (Oluwadere and Oyewumi, 2018; Edet and Ikot, 2021) as presented in Table 1, also adopted the conversion $\hbar c = 1973.29\ \text{eV}\,\mathring{A}$ by Okon, *et al*.,(2018), we computed the vibrational energies of HSKP for CuLi, TiH, VH, TiC, HCl, LiH, H_2, ScH, CO , I_2 , N_2 and NO diatomic molecules as shown in Tables 2-4. It is observed that for each vibrational quantum number, the vibrational energies increases with an increase in the rotational quantum number, for each of the selected diatomic molecules. Also, using Eqs. (31) and (33),we computed the bound state energy for HCl and LiH diatomic molecules, it was noticed to be in good agreement with the report of Ibekwe *et al*.,(2021) and Ikot *et al*.,(2019) as shown in Table 5-7. In Figs. 1-3, we plotted the energy eigenvalues of HSKP for selected molecules for different rotational quantum numbers (RQN). Figure 1 show an increase with increasing principal quantum number for different values of rotational quantum number l, then later, a sharp decrease is noticed. The plot of the energy eigenvalues of HCl and LIH with different values of rotational quantum number is shown in Fig 2 and Fig. 3. It depicts a monotonic decrease as the PQN increases.

Table 1. Spectroscopic data of the selected diatomic molecules used in this study (Oluwadere and Oyewumi, 2018; Edet and Ikot,2021)

Molecules	$D_e\left(\mathrm{eV}\right)$	$\alpha^{-\vartheta}\left(\overset{\circ}{\mathrm{A}}^{-1}\right)$	$r_e\left(\overset{\&}{\mathrm{A}}\right)$	$\mu\left(\mathrm{MeV}\right)$
VH	2.3300000000	1.44370	1.7190	0.09203207571
TiH	2.0500000000	1.32408	1.7810	0.09197301899
TiC	2.6600000000	1.52550	1.7900	0.89480052210
CuLi	1.7400000000	1.00818	2.3100	0.58306812790
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
ScH	2.2500000000	1.41130	1.7760	0.09184903714
CO	11.225600000	2.29940	1.1283	0.63906749030
I_2	1.5556000000	1.86430	2.6620	5.91053779800
N_2	11.938190000	2.69860	1.0940	0.65235787010
NO	8.0437300000	1.86430	1.1508	5.91053826200

Table 2. Bound state energy $E_{nl}\left(\mathrm{eV}\right)$ spectra of HSKP for VH, TiH, TiC and CuLi diatomic molecules

n	l	**VH**	**TiH**	**TiC**	**CuLi**
0	0	-11.70055424	-9.726651786	-14.87214595	-8.132246170
0	1	-11.70046448	-9.726603877	-14.87212745	-8.132242543
0	2	-11.70028531	-9.726508227	-14.87209046	-8.132235296
0	3	-11.70001734	-9.726365207	-14.87203497	-8.132224424
0	4	-11.69966155	-9.726175348	-14.87196103	-8.132209934
0	5	-11.69921917	-9.725939356	-14.87186864	-8.132191834
1	0	-11.75133279	-9.761604839	-14.89612085	-8.140341389
1	1	-11.75123363	-9.761549947	-14.89610195	-8.140337540
1	2	-11.75103566	-9.761440365	-14.89606416	-8.140329849
1	3	-11.75073954	-9.761276477	-14.89600750	-8.140318316
1	4	-11.75034627	-9.761058867	-14.89593198	-8.140302940

1	5	-11.74985720	-9.760788298	-14.89583762	-8.140283740
2	0	-11.80817248	-9.801994722	-14.92074289	-8.148966335
2	1	-11.80806518	-9.801933825	-14.92072362	-8.148962273
2	2	-11.80785095	-9.801812245	-14.92068507	-8.148954157
2	3	-11.80753048	-9.801630393	-14.92062727	-8.148941990
2	4	-11.80710481	-9.801388884	-14.92055022	-8.148925773
2	5	-11.80657534	-9.801088529	-14.92045397	-8.148905512
3	0	-11.87082065	-98475804151	-14.94600429	-8.158112570
3	1	-11.87070648	-9.847514496	-14.94598464	-8.158108311
3	2	-11.87047852	-9.847382873	-14.94594536	-8.158099787
3	3	-11.87013748	-9.847185978	-14.94588647	-8.158087016
3	4	-11.86968442	-9.846924452	-14.94580797	-8.158069994
3	5	-11.86912079	-9.846599150	-14.94570987	-8.158048718
4	0	-11.93904501	-9.898140839	-14.97189741	-8.167771911
4	1	-11.93892522	-9.898070872	-14.97187742	-8.167767459
4	2	-11.93868602	-9.897931165	-14.97187742	-8.167758554
4	3	-11.93832814	-9.897722157	-14.97177750	-8.167745198
4	4	-11.93785265	-9.897444504	-14.97169760	-8.167727407
4	5	-11.93726103	-9.897099094	-14.97159775	-8.167705175
5	0	-12.01263170	-9.953472901	-14.99841485	-8.177936405
5	1	-12.01250752	-9.953399865	-14.99839452	-8.177931769
5	2	-12.01225953	-9.953254017	-14.99835387	-8.177922505
5	3	-12.01188847	-9.953035813	-14.99829292	-8.177908598
5	4	-12.01139544	-9.952745913	-14.99821167	-8.177890068
5	5	-12.01078190	-9.952385224	-14.99811015	-8.177866915

Table 3. Bound state energy spectra $E_{nl}\left(eV\right)$ of HSKP for HCl, LiH, H_2 and ScH diatomic molecules

n	*l*	**HCl**	**LiH**	**H_2**	**ScH**
0	0	-22.17032494	-9.044861721	-13.92974441	-11.42415689
0	1	-22.17022128	-9.044847651	-13.93464244	-11.42406419
0	2	-22.17001432	-9.044819582	-13.94456401	-11.42387908
0	3	-22.16970474	-9.044777634	-13.94456401	-11.42360222
0	4	-22.16929354	-9.044722014	-13.98060726	-11.42323457
0	5	-22.16878209	-9.044652964	-13.98060745	-11.42277740
1	0	-22.24690799	-9.033844252	-13.79739618	-11.47486957
1	1	-22.24679078	-9.033836790	-13.80084636	-11.47476776
1	2	-22.24655670	-9.033821914	-13.80786295	-11.47456447
1	3	-22.24620649	-9.033799708	-13.81867833	-11.47426038
1	4	-22.24574126	-9.033770284	-13.83364106	-11.47385650
1	5	-22.24516244	-9.033733821	-13.85321597	-11.47335416
2	0	-22.33432382	-9.029306244	-13.70661022	-11.53131814
2	1	-22.33419477	-9.029304880	-13.70872277	-11.53120845
2	2	-22.33393705	-9.029302176	-13.71305549	-11.53098942
2	3	-22.33355145	-9.029298171	-13.71982357	-11.53066173

2	4	-22.33303911	-9.029292928	-13.72934979	-11.53022644
2	5	-22.33240157	-9.029286529	-13.74206457	-11.52968494
3	0	-22.43212310	-9.030892408	-13.65662021	-11.52968449
3	1	-22.43198398	-9.030896786	-13.65749846	-11.59315190
3	2	-22.43198398	-9.030905540	-13.65935463	-11.59291951
3	3	-22.43129039	-9.030918685	-13.66238806	-11.59257183
3	4	-22.43073793	-9.030936216	-13.66689774	-11.59210992
3	5	-22.43005037	-9.030958150	-13.67328236	-11.59153520
4	0	-22.53989148	-9.038278642	-13.64667365	-11.66050422
4	1	-22.53974404	-9.038288540	-13.64641418	-11.66038236
4	2	-22.53944960	-9.038308324	-13.64598762	-11.66013900
4	3	-22.53900894	-9.038337960	-13.64557866	-11.65977486
4	4	-22.53842333	-9.038377402	-13.64546438	-11.65929105
4	5	-22.53769441	-9.038426596	-13.64601419	-11.65929105
5	0	-22.65724630	-9.051168821	-13.67603704	-11.73282718
5	1	-22.65709229	-9.051184136	-13.67472988	-11.73270100
5	2	-22.65678471	-9.051214731	-13.67220119	-11.73244899
5	3	-22.65632439	-9.051260542	-13.66862223	-11.73207189
5	4	-22.65571258	-9.051321485	-13.66424984	-11.73157080
5	5	-22.65495095	-9.051397418	-13.65942655	-11.73094716

Table 4. Bound state energy spectra $E_{nl}\left(eV\right)$ of HSKP for CO, I2, N2 and NO diatomic molecules

n	*l*	**CO**	**I_2**	**N_2**	**NO**
0	0	-59.25288028	-18.85027835	-73.23970978	-34.53518839
0	1	-59.25250501	-18.85025791	-73.23959572	-34.53518812
0	2	-59.25175467	-18.85021699	-73.23936765	-34.53518756
0	3	-59.25062968	-18.85015564	-73.23902562	-34.53518674
0	4	-59.24913067	-18.85007384	-73.23856971	-34.53518565
0	5	-59.24725845	-18.84997158	-73.23800004	-34.53518429
1	0	-59.32596985	-18.87811728	-73.37100834	-34.53969898
1	1	-59.32592581	-18.87809681	-73.37089269	-34.53969869
1	2	-59.32583776	-18.87805588	-73.37066144	-34.53969812
1	3	-59.32570568	-18.87799448	-73.37031465	-34.53969726
1	4	-59.32552965	-18.87791264	-73.36985235	-34.53969611
1	5	-59.32530968	-18.87781033	-73.36927468	-34.53969468
2	0	-59.40126038	-18.90604095	-73.50484846	-34.54441426
2	1	-59.40121530	-18.90602048	-73.50473127	-34.54441398
2	2	-59.40112517	-18.90597952	-73.50449695	-34.54441337
2	3	-59.40098997	-18.90591811	-73.50414554	-34.54441248
2	4	-59.40080973	-18.90583620	-73.50367709	-34.54441128
2	5	-59.40058454	-18.90573384	-73.50309178	-34.54440980
3	0	-59.47872659	-18.93404920	-73.64120398	-34.54933324
3	1	-59.47868051	-18.93402872	-73.64108535	-34.54332920

3	2	-59.47858833	-18.93398774	-73.64084805	-34.54933232
3	3	-59.47845012	-18.93392687	-73.64049220	-34.54933137
3	4	-59.47826584	-18.93384435	-73.64001786	-34.54933014
3	5	-59.47803559	-18.93374193	-73.63942518	-34.54932858
4	0	-59.55834376	-18.96214182	-73.78004941	-34.54932858
4	1	-59.55829667	-18.96212133	-73.77992938	-34.55445454
4	2	-59.55820256	-18.96208034	-73.77968920	-34.55445388
4	3	-59.55806138	-18.96201886	-73.77932912	-34.55445292
4	4	-59.55787323	-18.96193686	-73.77884909	-34.55441620
4	5	-59.55763814	-18.96183440	-73.77824929	-34.55445003
5	0	-59.55763814	-18.99031865	-73.92135979	-34.55977811
5	1	-59.64003961	-18.99029814	-73.92123836	-34.55977778
5	2	-59.63994361	-18.99025714	-73.92099551	-34.55977710
5	3	-59.63994361	-18.99019562	-73.92063132	-34.55977611
5	4	-59.63979964	-18.99019562	-73.92014586	-34.55977476
5	5	-59.63960774	-18.99001108	-73.91953921	-34.55977310

Table 5: Comparison of the Energy eigenvalues of the Kratzer potential for HCl

n	l	**Present work**	**Ibekwe *et al.*, 2021**	**Ikot *et al.*, 2019**
0	0	-4.54184821	-4.574322886	-4.541847882
1	0	-4.39372795	-4.402122552	-4.393727024
	1	-4.39129385	-4.401308521	-4.391292904
2	0	-4.25273711	-4.239466022	-4.252735636
	1	-4.25041920	-4.238696688	-4.250417718
	2	-4.24579105	-4.237158875	-4.245789526
3	0	-4.11842537	-4.085660853	-4.118423404
	1	-4.11621638	-4.084933001	-4.116214408
	2	-4.11180563	-4.083478096	-4.111803616
	3	-4.10520744	-4.081297704	-4.105205380
4	0	-3.99037742	-3.940076275	-3.990375014
	1	-3.98827064	-3.939386976	-3.988268222
	2	-3.98406387	-3.938009125	-3.984061424
	3	-3.97777065	-3.935944185	-3.977768152
	4	-3.96941113	-3.933194375	-3.969408570
5	0	-3.86820974	-3.802136724	-3.868206938
	1	-3.86619896	-3.801483303	-3.866196140
	2	-3.86218380	-3.800177161	-3.862180950
	3	-3.85617703	-3.798219664	-3.856174134
	4	-3.84819767	-3.795612890	-3.848194720
	5	-3.83827087	-3.792359570	-3.838267840

Table 6: Comparison of the Energy eigenvalues of the Kratzer potential for LiH

n	*l*	**Present work**	**Ibekwe *et al.*, 2021**	**Ikot *et al.*, 2019**
0	0	-2.46731030	-2.467293680	-2.467293778
1	0	-2.37581921	-2.380989203	-2.375802636
	1	-2.37410797	-2.380416619	-2.374091378
2	0	-2.28932426	-2.281213703	-2.289307674
	1	-2.28770560	-2.280676728	-2.287688996
	2	-2.28447521	-2.279603547	-2.284458584
3	0	-2.20746820	-2.187580925	-2.207451626
	1	-2.20593555	-2.187076666	-2.205918968
	2	-2.20287674	-2.186068862	-2.202860140
	3	-2.19830467	-2.184558925	-2.198288040
4	0	-2.12992512	-2.099596786	-2.129908602
	1	-2.12847251	-2.099122640	-2.128455976
	2	-2.12557335	-2.098175007	-2.125556792
	3	-2.12123970	-2.096755197	-2.121223116
	4	-2.11548950	-2.094865172	-2.115472884
5	0	-2.05639728	-2.016815899	-2.056380834
	1	-2.05501922	-2.016369515	-2.055002762
	2	-2.05226878	-2.015477357	-2.052252304
	3	-2.04815726	-2.014140642	-2.048140758
	4	-2.04270146	-2.012361189	-2.042684928
	5	-2.03592352	-2.010141421	-2.035906942

Table7: Comparison of the Energy of the screened Kratzer potential for HCl and LiH

n	*l*	**Present work for LiH**	**Present work for HCl**	**LiH (Ikot *et al.*, 2019)**	**HCl(Ikot *et al.*, 2019)**
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

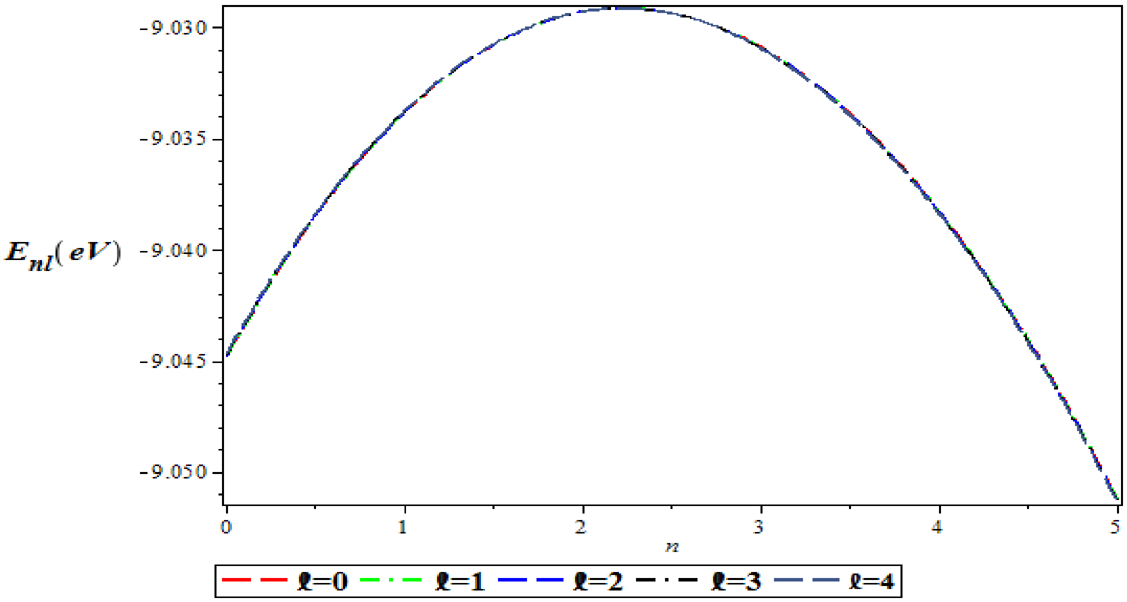

Fig. 1. Variation of the energy spectra for various l as a function of n for LiH Diatomic molecules

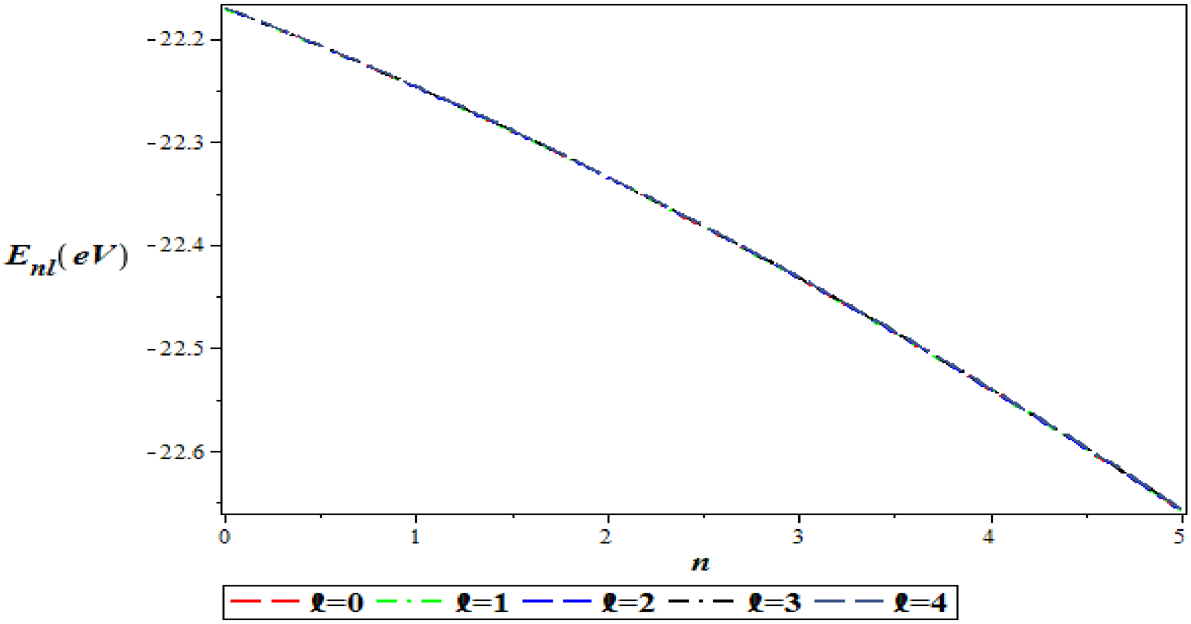

Fig 2. Variation of the energy spectra for various l as a function of n for HCl diatomic molecules

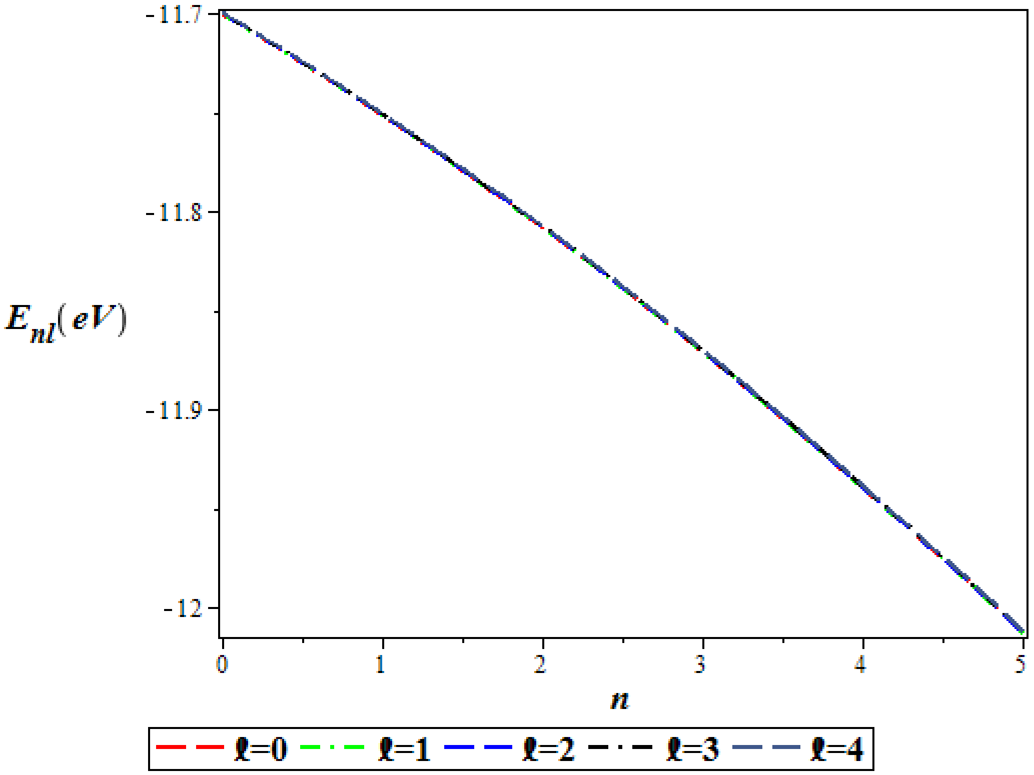

Fig 3. Variation of the energy spectra for various l as a function of n for VH Diatomic molecules

6.0 Conclusion

In this study, the solutions to the SE with HSKP have been obtained using the series expansion method. The application of the energy equation to study twelve (12) diatomic molecules revealed that bound state energy spectra of these diatomic molecules increases as various quantum numbers n and l increases. Computation of the bound state eigenvalues for two diatomic molecules using Kratzer potential and screened Kratzer potential were in good agreement with the report of other researchers in literature.

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