



Eigen Solutions of Schrodinger Equation with Screened-Kratzer-Eckart Potential (SKEP) Model in Higher Dimensions for Hydrogen-Related Diatomic Molecules

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Abstract

The screened-Kratzer-Eckart potential (SKEP) model is known to be a very effective potential model due to its combined effort in predicting the behaviour of diatomic molecules. The aim of this research is to study the variation of the energy eigenvalues of some hydrogen-related diatomic molecules with different spectroscopic parameters, both numerically and graphically. By employing the Nikiforov-Uvarov functional analysis (NUFA) method, the radial Schrodinger equation with the SKEP model was solved. The analytical expressions of the energy eigenvalues and un-normalized wave function were obtained in closed forms. Variations of energy eigenvalues with quantum numbers and spectroscopic parameters, with respect to selected hydrogen-related molecules were discussed extensively. Our numerical and graphical considerations show that the energies of SKEP depend strongly on the quantum states of the diatomic molecules, as well as their spectroscopic parameters.

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1.0 Introduction

It is well known that many potential energy models have been investigated to obtain information concerning the diatomic structures (Yanar *et al.*, 2016). Also, the recent studies of the relativistic and non-relativistic wave equations have attracted the attention of many authors because of the solutions these equations play in different aspects of physics (Ikot *et al.*, 2014).

For non-relativistic quantum mechanics, the radial solutions of Schrödinger equation (SE) are of great significance because the needed information to delineate a quantum system can be rooted in the wave function (Dong *et al.*, 2016; Ikot *et al.*, 2020). Since the birth of quantum mechanics, the non-relativistic solution of SE has drawn much attention, especially in studying exact solvable physical problems in different branches of Physics, of which, the applications of quantum mechanics are not limited to but incorporate molecular Physics, information theory, nuclear and particle physics (Edet *et al.*, 2020; Horchani *et al.*, 2021; Ibekwe *et al.*, 2021). In particular, this solution approach has been adopted in many studies to report the mass spectra, thermodynamic functions, transition properties and decay rates, as well as the binding energies of Physical systems of interest (Hadizadeh and Khaledi-nasab, 2016; Shalchi and Hadizadeh, 2016; Okorie *et al.*, 2018a; Ikot *et al.*, 2019; Sahraeian and Hadizadeh, 2019; Ibekwe *et al.*, 2020).

Different analytical techniques have been used by different authors to obtain the solutions of the wave equations with different quantum systems in their respective regimes. They include factorization method (Dong, 2007), Nikiforov-Uvarov (NU) method (Nikiforov and Uvarov, 1988), asymptotic iteration method (AIM) (Ciftci *et al.*, 2005; Bayrak *et al.*, 2007), NU Functional Analysis (NUFA) method (Ikot *et al.*, 2021), exact and proper quantization rule

(Qiang and Dong, 2010; Serrano *et al.*, 2011), super-symmetric quantum mechanics approach (Witten, 1981), extended Nikiforov-Uvarov (ENU) method (Karayer *et al.*, 2015a; Karayer *et al.*, 2015b), amongst others.

In recent times, the diatomic molecular potential models within the framework of three- and D-dimensional systems of Schrodinger equation (SE), Dirac equation (DE) and Klein-Gordon equation equation (KGE) have been studied (Jia *et al.*, 2014; Jia *et al.*, 2015). Antia *et al.* (2013) considered the KGE with equal scalar and vector Mobius square plus Yukawa potentials in D-dimensions, with the help of the parametric NU method. The D-dimensional SE with a combination of Coulomb potential and inverse trigonometry Scarf-type potential was studied by Onate and his collaborators (2018). Specific consideration was the application of their eigen solutions to evaluating onicescus information energy in higher dimensions. The solution of the D-dimensional KGE for multiparameter exponential-type potential has been obtained via the super-symmetric quantum mechanics approach (Ikot *et al.*, 2015). With the use of the modified factorization method, the energy eigenvalues and wave function of quadratic exponential-type potential (QEP) have been obtained in higher dimensions (Okorie *et al.*, 2018b). In that study, some thermal properties of QEP were calculated for Rubidium dimer. In another development, the nonrelativistic rotation-vibrational energies of nitrogen monoxide and hydrogen dimer have been investigated for their improved Rosen-Morse potential in D-dimensions (Udoh *et al.*, 2019). Okorie *et al.* (2019) solved the D-dimensional KGE with generalized hyperbolic potential with equal scalar and vector potential conditions, using functional analysis formalism. Relativistic and nonrelativistic ro-vibrational energies were obtained for different diatomic molecules, and inter-dimensional degeneracy symmetries were found to exist in the energies obtained.

In this paper, we intend to investigate the eigen solution variation of the screened-Kratzer-Eckart potential (SKEP), defined as

$$V(r) = \gamma \left(1 - \frac{g e^{-\delta r}}{1 - e^{-\delta r}} \right)^2 - \zeta \left(\frac{A}{r} - \frac{B}{2r^2} \right) e^{-\delta r}, \quad (1)$$

$$g \equiv (e^{\delta r_e} - 1), \quad A \equiv r_e, \quad B \equiv r_e^2, \quad \gamma \equiv d_e, \quad \zeta \equiv 2d_e$$

where d_e is the dissociation energy, r_e is the equilibrium bond length, r is the inter-atomic distance and δ is the screening parameter. The eigen solution, expectation values and thermodynamic properties of the screened Kratzer potential have been recently investigated (Ikot et al., 2019). Also, the Eckart potential has been applied in studies involving different wave equations, with the help of the above mentioned approximate method (Diao et al., 2009; Gao and Zhang, 2016; Sargolzaeipor et al., 2018a; Sargolzaeipor et al., 2018b). The combination of the screened Kratzer potential and the Eckart potential is to achieve a wider applicability, which has not been studied before, to the best of our knowledge.

In view of this development, the aim of this research is to study the variation of the energy eigenvalues of some hydrogen-related diatomic

molecules with different spectroscopic parameters, both numerically and graphically. This article is organized as follows: In section 2, a review of the Nikiforov-Uvarov functional analysis (NUFA) method is presented. The solutions of the Schrodinger equation with SKEP in D-dimensions are presented in section 3. In section 4, the results obtained are presented and discussed accordingly. The concluding remarks are presented in section 5.

2.0 Materials and Method

2.1 Review of Nikiforov – Uvarov Functional Analysis (NUFA) Method

Ikot et al. (2021) proposed a method for solving a second order differential equation of the hyper geometric type. Also the NU is used to solve a second order differential equation of the form (Nikiforov and Uvarov, 1988)

$$\psi_n''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)} \psi_n'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)} \psi_n(s) = 0 \quad (2)$$

where $\sigma(s)$ and $\tilde{\sigma}$ are polynomials, at most of second degree, and $\tilde{\tau}(s)$ is a first-degree polynomial. Tezcan and Sever (2009) introduced the parametric form of NU method in the form

$$\psi''(s) + \frac{\alpha_1 - \alpha_2 s}{s(1 - \alpha_3 s)} \psi'(s) + \frac{1}{s^2(1 - \alpha_3 s)^2} [-\xi_1 s^2 + \xi_2 s - \xi_3] \psi(s) = 0 \quad (3)$$

where α_i and $\xi_i (i=1,2,3)$ are all parameters. It can be observed in equation (3) that the differential equation has two singularities at $s \rightarrow 0$ and $s \rightarrow \frac{1}{\alpha_3}$, thus we take the wave function in the form,

$$\psi(s) = s^\sigma (1 - \alpha_3 s)^\nu f(s) \quad (4)$$

Substituting equation (4) into equation (3) gives the following equation,

$$s(1-\alpha_3s)f''(s) + [\alpha_1 + 2\sigma - (2\sigma\alpha_3 + 2v\alpha_3 + \alpha_2)s]f'(s) - \alpha_3 \left(\sigma + v + \frac{\alpha_2}{\alpha_3} - 1 + \sqrt{\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 + \frac{\xi_1}{\alpha_3}} \right) \left(\sigma + v + \frac{\alpha_2}{\alpha_3} - 1 + \sqrt{\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 + \frac{\xi_2}{\alpha_3}} \right) + \left[\frac{\sigma(\sigma-1) + \alpha_1\sigma - \xi_3}{s} + \frac{\alpha_2v - \alpha_1\alpha_3v(v-1)\alpha_3 - \frac{\xi_1}{\alpha_3} + \xi_2 - \xi_3\alpha_3}{(1-\alpha_3s)} \right] \times f(s) = 0 \quad (5)$$

Equation (5) can be reduced to a Gauss hypergeometric equation if and only if the following functions vanished.

$$\sigma(\sigma-1) + \alpha_1\sigma - \xi_3 = 0 \quad (6)$$

$$\alpha_2v - \alpha_1\alpha_2v + v(v-1)\alpha_3 - \frac{\xi_1}{\alpha_3} + \xi_2 - \xi_3\alpha_3 = 0 \quad (7)$$

Thus, equation (5) becomes

$$s(1-\alpha_1s)f''(s) + [\alpha_1 + 2\sigma - (2\sigma\alpha_3 + 2v\alpha_3 + \alpha_2)s]f'(s) - \alpha_3 \left(\sigma + v + \frac{\alpha_2}{\alpha_3} - 1 + \sqrt{\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 + \frac{\xi_1}{\alpha_3}} \right) \left(\sigma + v + \frac{\alpha_2}{\alpha_3} - 1 + \sqrt{\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 + \frac{\xi_1}{\alpha_3}} \right) f(s) = 0 \quad (8)$$

By solving equations (6) and (7) result,

$$\sigma = \frac{(1-\alpha_1) \pm \sqrt{(1-\alpha_1)^2 + 4\xi_3}}{2} \quad (9)$$

$$v = \frac{(\alpha_3 + \alpha_1\alpha_3 - \alpha_2) \pm \sqrt{(\alpha_3 + \alpha_1\alpha_3 - \alpha_2)^2 + 4\left(\frac{\xi_1}{\alpha_3} + \alpha_3\xi_3 - \xi_2\right)}}{2} \quad (10)$$

According to Dong *et al.* (2014), Equation (8) is the hypergeometric equation type of the form:

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

By using equations (4), (8) and (11), we obtain the energy equation and the corresponding unnormalized wave equation, respectively, for the NUFA method as follows:

$$\sigma^2 + 2\sigma \left(v + \frac{\alpha_2}{\alpha_3} - 1 + \frac{n}{\sqrt{\alpha_3}} \right) + \left(v + \frac{\alpha_2}{\alpha_3} - 1 + \frac{n}{\sqrt{\alpha_3}} \right)^2 - \left(\frac{\alpha_2}{\alpha_3} - 1 \right)^2 - \frac{\xi_1}{\alpha_3} = 0 \quad (12)$$

$$\psi(s) = N_{nl} s^{\frac{(1-\alpha_1) + \sqrt{(1-\alpha_1)^2 + 4\xi_3}}{2}} (1-\alpha_3s)^{\frac{(\alpha_3 + \alpha_1\alpha_3 - \alpha_2) + \sqrt{(\alpha_3 + \alpha_1\alpha_3 - \alpha_2)^2 + 4\left(\frac{\xi_1}{\alpha_3} + \alpha_3\xi_3 - \xi_2\right)}}{2}} {}_2F_1(a, b, c : s) \quad (13)$$

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

$$a = \sqrt{\alpha_3} \left(\sigma + \nu + \frac{\alpha_2}{\alpha_3} - 1 + \sqrt{\left(\frac{\alpha_2}{\alpha_3} - 1 \right)^2 + \frac{\xi_1}{\alpha_3}} \right) \quad (14)$$

$$b = \sqrt{\alpha_3} \left(\sigma + \nu + \frac{\alpha_2}{\alpha_3} - 1 - \sqrt{\left(\frac{\alpha_2}{\alpha_3} - 1 \right)^2 + \frac{\xi_1}{\alpha_3}} \right) \quad (15)$$

$$c = a_1 + 2\mu \quad (16)$$

2.2 Solutions of D-Dimensional Schrodinger with SKEP

According to Hassanabadi *et al.* (2012), the Schrodinger equation in D-Dimension reads as:

$$\frac{d^2 R_{nl}(r)}{dr^2} + \frac{2\mu}{\hbar^2} (E_{nl} - V(r)) R_{nl}(r) - \frac{1}{r^2} \left[\frac{(D+2l-1)(D+2l-3)}{4} \right] R_{nl}(r) = 0 \quad (17)$$

where μ is the reduced mass, E_{nl} is the energy spectrum, \hbar is the reduced Plank's constant and n and l are the radial and orbital angular momentum quantum numbers, respectively.

Substituting equation (1) into equation (17) gives

$$\frac{d^2 R_{nl}(r)}{dr^2} + \frac{2\mu E_{nl}}{\hbar^2} - \frac{2\mu}{\hbar^2} \left[\gamma \left(1 - \frac{ge^{-\delta r}}{1-e^{-\delta r}} \right)^2 - \zeta \left(\frac{A}{r} - \frac{B}{2r^2} \right) e^{-\delta r} \right] - \frac{1}{r^2} \left[\frac{(D+2l-1)(D+2l-3)}{4} \right] R_{nl}(r) = 0 \quad (18)$$

By employing the approximation scheme (Greene and Aldrich, 1976; Zhang *et al.*, 2011)

$$\frac{1}{r^2} \approx \frac{\delta^2}{(1-e^{-\delta r})^2}; \quad \frac{1}{r} \approx \frac{\delta}{(1-e^{-\delta r})} \quad (19)$$

and using the coordinate transformation of the form, $s = e^{-\delta r}$, equation (18) reduces to the differential equation

$$\frac{d^2 R_{nl}}{ds^2} + \frac{(1-s)}{s(1-s)} \frac{dR_{nl}}{ds} + \frac{1}{s^2(1-s)^2} \left[-(\varepsilon^2 + \phi + Y)s^2 + (2\varepsilon^2 + \phi + T)s - \left(\varepsilon^2 + \frac{M}{4} \right) \right] R_{nl}(s) = 0 \quad (20)$$

where,

$$-\varepsilon^2 = \frac{2\mu E}{\hbar^2 \delta^2} - \frac{2\mu \gamma}{\hbar^2 \delta^2}, \quad M = (D+2l-1)(D+2l-3), \quad (21)$$

$$\phi = \frac{4\mu \gamma g}{\hbar^2 \delta^2} + \frac{2\mu \zeta A}{\hbar^2 \delta}, \quad Y = \frac{2\mu \gamma g}{\hbar^2 \delta^2}, \quad T = \frac{\mu \zeta B}{\hbar^2}$$

By comparing equations (20) and (3) gives

$$\alpha_1 = \alpha_2 = \alpha_3 = 1$$

$$\xi_1 = \varepsilon^2 + \phi + Y; \quad \xi_2 = 2\varepsilon^2 + \phi - T; \quad \xi_3 = \varepsilon^2 + \frac{M}{4} \quad (22)$$

By using equations (9), (10) and (21), we can obtain the values of σ and \square as follows

$$\sigma = \sqrt{\varepsilon^2 + \frac{M}{4}}$$

$$v = \frac{1}{2} + \frac{1}{2} \sqrt{1 + 4 \left(Y + \frac{M}{4} + T \right)}$$
(23)

The energy spectrum and the corresponding un-normalized wave equations are obtained from equations (12) and (13), respectively as follows:

$$E_{nl} = d_e + \frac{\hbar^2 \delta^2 M}{8\mu} - \frac{\hbar^2 \delta^2}{2\mu} \left[\frac{4\mu d_e (e^{\delta r_e} - 1)}{\hbar^2 \delta^2} + \frac{2\mu d_e (e^{\delta r_e} - 1)^2}{\hbar^2 \delta^2} + \frac{4\mu d_e r_e - M}{\hbar^2 \delta} - \frac{M}{4} - \frac{(n+v)}{2} \right]^2$$
(24)

$$R_{nl}(r) = N_{nl} (e^{-\delta r})^{\sqrt{\varepsilon^2 + \frac{M}{4}}} (1 - e^{-\delta r})^{\frac{1}{2} + \frac{1}{2} \sqrt{1 + 4 \left(\gamma + \frac{M}{4} + T \right)}} {}_2F_1(a, b, c; e^{-\delta r})$$
(25)

where $v = \frac{1}{2} \left[1 + \sqrt{1 + \frac{8\mu d_e (e^{\delta r_e} - 1)^2}{\hbar^2 \delta^2} + \frac{8\mu d_e r_e^2}{\hbar^2} + (D + 2l - 1)(D + 2l - 3)} \right]$

(26)

3.0 Results and Discussion

In this work, the D-dimensional radial Schrodinger equation is solved with the SKEP of Eq. (1) in closed form and the energy eigen-solutions is obtained analytically using NUFA method as expressed in Eqs. (24) and (25), respectively. Numerical results of the energy eigenvalues for some hydrogen-related diatomic molecules (H_2 , HCl and LiH) are obtained and displayed in Table 2 using the spectroscopic parameters in Table 1 (Oyewumi et al., 2013). The numerical results depicted in Table 2 for the selected diatomic molecules are presented for various orbital and angular momentum quantum numbers. The following conversion units have been adopted in our computations (Oyewumi *et al.*, 2014):

$\hbar c = 1973.269 \text{ eV \AA}$ and $1 \text{ amu} = 9.31494028 \text{ MeVc}^{-2}$. It is also observed in Table 2 that the energy of the system for all three molecules increases as the orbital momentum quantum number l is increased for a fixed quantum

number n . Also, there is an increase in the energy of the diatomic molecule systems as the

dimension D , increases for a fixed quantum state. The effects of potential parameters on the energy eigenvalues of SKEP on the hydrogen-related diatomic molecules were investigated and presented in figures 1(a – f) respectively. Clearly, it can be seen that the dissociation energy d_e , the screening parameter δ , the dimensionality parameter D , as well as the angular momentum quantum number l , exhibit similar characteristics with regards to energy eigenvalues variations. However, the energy eigenvalues increase with increasing d_e , δ , D and l , respectively as shown in figures 1(a), 1(c), 1(d) and 1(f), for various diatomic molecules. In figure 1(b), the energies decrease first for small enhancement of the equilibrium bond length, r_e . Further enhancement of r_e results in increase in the energies of the diatomic molecules. As the equilibrium bond length is increased the more, the energies of the selected diatomic molecules decreases

and then remains constant at unique values. Figure 1(e) shows a monotonous decrease in energies with increase in orbital quantum number n , for the various diatomic molecules. A close observation from figures 1(a – f) showed that the bound state energy of SKEP is highly sensitive to the spectroscopic parameters

and different quantum numbers. Our studies can be readily applied to statistical physics and molecular physics (Valencia-Ortega and Arias-Hernandez, 2018; Chen et al., 2019; Jia et al., 2019; Jiang et al., 2019; Khordad and Ghambari, 2019; Khordad et al., 2019; Chabi and Boumali, 2020; Tang et al., 2020).

Table 1: Spectroscopic parameters for the selected diatomic molecules (Qiang and Dong, 2010)

Molecules	d_e (eV)	r_e (Å)	δ (Å ⁻¹)	μ (a.m.u)
H_2	4.7446	0.7416	1.9426	0.050391
HCl	4.6190	1.2746	1.8677	0.980105
LiH	2.5152	1.5956	1.1280	0.880122

Table 2: Ro-vibrational energy eigenvalues of the SKEP for H_2 molecule at different dimensions

n	l	$E_{nl}^{D=3}$	$E_{nl}^{D=4}$	$E_{nl}^{D=5}$
0	0	0.093966783	0.113175070	0.145172061
1	0	0.751917178	0.770454075	0.801332922
	1	0.801332922	0.844529801	0.900112580
2	0	1.348679452	1.366579027	1.396396451
	1	1.396396451	1.438108960	1.491684736
	2	1.491684736	1.557082976	1.634254009
3	0	1.887513428	1.904807357	1.933616101
	1	1.933616101	1.973917985	2.025682708
	2	2.025682708	2.088871428	2.163436842
	3	2.163436842	2.249323223	2.346466537

Table 3: Ro-vibrational energy eigenvalue of the SKEP for HCl molecule at different dimensions

n	l	$E_{nl}^{D=3}$	$E_{nl}^{D=4}$	$E_{nl}^{D=5}$
0	0	0.835701454	0.842324632	0.853362978
1	0	1.191668876	1.198237640	1.209185272
	1	1.209185272	1.224511265	1.244214825
2	0	1.528651154	1.535166158	1.546024214
	1	1.546024214	1.561224789	1.580767102
	2	1.580767102	1.604650300	1.632873288
3	0	1.846887161	1.853349082	1.864118649
	1	1.864118649	1.879195333	1.898578367
	2	1.898578367	1.922266934	1.950259948

	3	1.950259948	1.982555991	2.019153628
Table 4: Ro-vibrational energy eigenvalue of the SKEP for <i>LiH</i> molecule at different dimensions				
<i>n</i>	1	$E_{nl}^{D=3}$	$E_{nl}^{D=4}$	$E_{nl}^{D=5}$
0	0	0.2209776820	0.2241218880	0.2293618060
1	0	0.4121935740	0.4152945900	0.4204625140
	1	0.4204625140	0.4276966870	0.4369962360
2	0	0.5937847740	0.5968434620	0.6019408530
	1	0.6019408530	0.6090763020	0.6182489630
	2	0.6182489630	0.6294576660	0.6427010540
3	0	0.7659558360	0.7689730530	0.7740013510
	1	0.7740013510	0.7810400680	0.7900883880
	2	0.7900883880	0.8011451620	0.8142090580
	3	0.8142090580	0.8292784840	0.8463515660

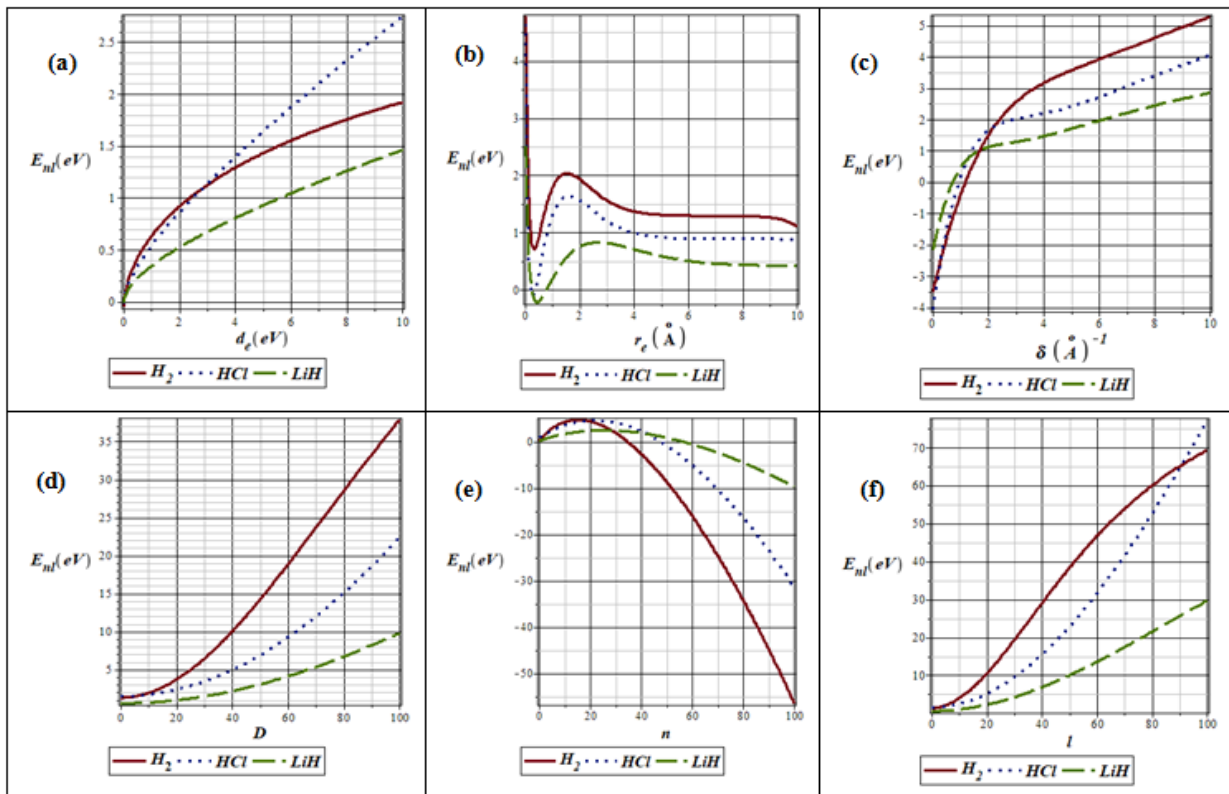


Figure 1: Variation of Energy eigenvalues of SKEP with different spectroscopic parameters and quantum numbers for selected hydrogen-related molecules

4.0 Conclusion

In this paper, we obtained the bound state solutions of the radial Schrodinger equation

with the screened-Kratzer-Eckart potential (SKEP) in D-dimensions using the Nikiforov-Uvarov functional analysis (NUFA) method.

The energy eigenvalues and the un-normalized wave function of SKEP were obtained accordingly. Numerical and graphical variations of the energies of SKEP with quantum numbers and spectroscopic parameters were evaluated and discussed, with respect to selected hydrogen-related diatomic molecules. Our analysis shows that the energies of SKEP depend on the quantum numbers and spectroscopic parameters of the selected molecules, and our studies can be applied to statistical and molecular physics.

Data Availability Statement

Data will be available on request.

Conflict of Interest Declaration

The authors declare that there are no conflicts of interest among them, as regards this article. Thank you.

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