Volume 15, Number 2, 2022. pp. 179-193

Jordan Journal of Physics

ARTICLE

Solutions of the Non-relativistic Equation Interacting with the Varshni-Hellmann Potential Model with Some Selected Diatomic Molecules

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Doi: **https://doi.org/10.47011/15.2.8**

Received on: 13/11/2020; Accepted on: 01/02/2021

Abstract: The approximate solutions of Schrödinger equation for the newly proposed Varshni-Hellmann potential (VHP) are obtained within the framework of the Nikiforov-Uvarov method by employing the Greene-Aldrich approximation scheme to deal with the centrifugal term. The numerical results of the ro-vibrational energies and normalized wavefunction in closed form are obtained in terms of Jacobi polynomials for various quantum states of the diatomic molecules of LiH, TiH, CrH and ScN, respectively. Four special cases of the potential are also studied and their numerical energy eigenvalues evaluated are in agreement with those reported in the existing literature. Also, the behavior of the energy spectra for the ground state of the selected diatomic molecules is illustrated graphically.

Keywords: Schrödinger equation; Varshni-Hellmann potential, Nikiforov-Uvarov method, Diatomic molecules.

1. Introduction

The exact and approximate solutions of quantum wave equations like Schrödinger, Lippmann-Schwinger, Klein-Gordon and Dirac equations, have been a striking research area under discussion in physics, chemistry and applied mathematics [1-4]. The Schrödinger equation is a second-order differential equation used in solving quantum mechanical problems [5]. The eigenvalues and wave functions contain considerable information about quantum systems, such as atomic structure, quantum electrodynamics and vibrations in molecules [6-9]. The wave functions and their equivalent eigenvalues give considerable information on describing different quantum systems, such as the atomic structure theory, quantum-chemical theory, quantum electrodynamics theory and theory of molecular vibrations [6-9]. With the experimental proof of the Schrödinger wave equation, researchers have dedicated much attention to solving the radial Schrödinger equation with different analytical methods to obtain approximate bound-state solutions for some physical potential models, such as Yukawa potential [10], Wood-Saxon potential [11], Eckart potential [12], generalized Morse potential [13], Makorov potential [14], Hulthen potential [15], Hellmann potential [16], … etc., by using certain approximation schemes. The most widely used approximation was introduced by Pekeris [17] and another form was suggested by Greene and Aldrich [18].

Efforts have been made by many researchers to solve the Schrödinger and Klein-Gordon equations by the superposition of different potentials, which can be used for a wider range of applications [19, 20]. For example, William et al. studied Hulthen potential together with

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Hellmann potential [21], Ahmadov et al. solved the Klein-Gordon equation by Manning-Rosen plus a class of Yukawa potentials [22], Manning-Rosen potential plus a ring-shaped like potential [23], Aspoukeh and Hamad studied the Klein-Gordon equation for vector and scalar Hellmann plus modified Kratzer potentials [24] and Hans Hellmann investigated the Schrödinger equation with a linear combination of Coulomb and Yukawa potential, which is called Hellmann potential [25]. The Hellmann potential has been applied to several branches in physics, such as atomic physics, plasma physics, solid-state physics, … etc. [26–30], as well as in the study of electron-core [31], electron-ion [32] and inner-shell ionization problems and alkali hydride molecules [33]. The bound-state energy eigenvalues have been obtained by other researchers in Refs. [34-41]. The Hellmann potential is of the form [25, 42-46]:

$$V(r) = -\frac{c}{r} + \frac{de^{-\beta r}}{r} \tag{1}$$

where r is the inter-nuclear distance, c , and d are the strengths of Coulomb and Yukawa potentials and β is the screening parameter. The Varshni potential is of the form [47]:

$$V(r) = a\left[1 - \frac{b}{r}e^{-\beta r}\right] \tag{2}$$

where a and b are the strengths of the Varshni potential, respectively and β is the screening parameter which controls the shape of the potential energy curve. Varshni potential is a short-range repulsive potential energy function which has been investigated within the formalism of the Schrödinger equation and plays a fundamental role in chemical and molecular physics. Many authors have worked on this potential, such as in Refs. [48, 49].

In this study, we attempt to study the radial Schrödinger equation with a newly proposed potential obtained by the superposition of Varshni and Hellmann potential (VHP). The potential is of the form:

$$V(r) = a - \frac{abe^{-\beta r}}{r} - \frac{c}{r} + \frac{de^{-\beta r}}{r}. \tag{3}$$

The shape of this potential as a function of inter-nuclear distance of LiH, TiH, CrH and ScN diatomic molecules is presented in Fig. 1.

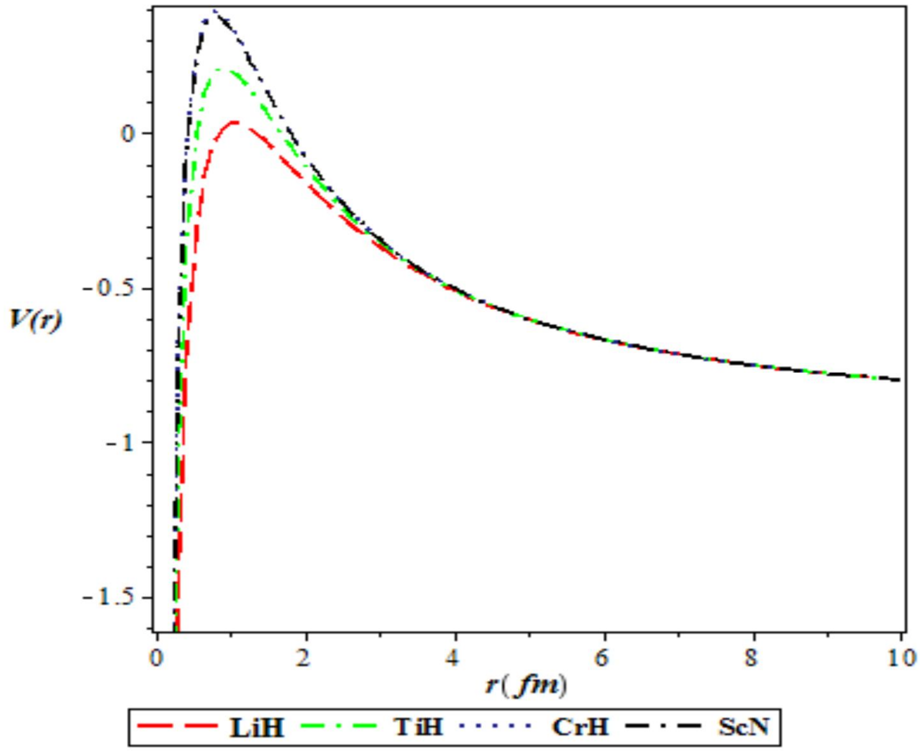

FIG. 1. Variation of Varshni plus Hellmann potential as a function of r for the selected diatomic molecules.

2. Bound-state Solutions of the Schrödinger Equation with VHP

The radial part of the Schrödinger equation is given by [50, 51]:

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

where μ is the reduced mass, E_{nl} is the energy spectrum to be determined, $\hbar$ is the reduced Planck's constant, r is the inter-particle distance, $V(r)$ is the interacting potential, $\frac{\ell(\ell+1)}{r^2}$ is the centrifugal term and n and l are the radial and orbital angular momentum quantum numbers, respectively. In solving Eq.(4) analytically, we introduce the Greene-Aldrich approximation scheme [18,52] to deal with the centrifugal barrier. This approximation scheme is a good approximation to the centrifugal barrier which is valid for $\beta << 1$ and is given as:

$$\frac{1}{r^2} \approx \frac{\beta^2}{\left(1-e^{-\beta r}\right)^2}. \tag{5}$$

Substituting Eq. (3) and Eq. (5) into Eq. (4), we have:

$$\frac{d^2R_{nl}(r)}{dr^2} + \left[\frac{2\mu}{\hbar^2}\left(E_{nl} - a + \frac{ab\beta e^{-\beta r}}{(1-e^{-\beta r})} + \frac{c\beta}{(1-e^{-\beta r})} - \frac{d\beta e^{-\beta r}}{(1-e^{-\beta r})}\right) - \frac{\beta^2 l(l+1)}{(1-e^{-\beta r})^2}\right]R_{nl}(r) = 0. \tag{6}$$

By using coordinate transformation:

$$x = e^{-\beta r}. \tag{7}$$

we obtain the differential equation of the form:

$$\frac{d^2R(x)}{dx^2} + \frac{1-x}{x(1-x)}\frac{dR(x)}{dx} + \frac{1}{x^2(1-x)^2}\left[-(\varepsilon+\varsigma_0)x^2 + (2\varepsilon+\varsigma_0-\varsigma_1)x - (\varepsilon-\varsigma_1+\gamma)\right]R(x) = 0 \tag{8}$$

where

$$-\varepsilon = \frac{2\mu E_{nl}}{\hbar^2\beta^2} - \frac{2a\mu}{\hbar^2\beta^2}, \varsigma_0 = \frac{2ab\mu}{\hbar^2\beta} - \frac{2d\mu}{\hbar^2\beta}, \varsigma_1 = \frac{2c\mu}{\hbar^2\beta}, \gamma = l(l+1). \tag{9}$$

Comparing Eqs. (8) and (A1),we have the following parameters:

$$\tilde{\sigma}(x) = -(\varepsilon+\varsigma_0)x^2 + (2\varepsilon+\varsigma_0-\varsigma_1)x - (\varepsilon-\varsigma_1+\gamma), \sigma(x) = x(1-x), \tilde{\tau}(x) = 1 - x\}. \tag{10}$$

Substituting Eq. (10) into Eq. (A9), we obtain:

$$\pi(x) = -\frac{x}{2} \pm \sqrt{(A-k)x^2 + (k+B)x + C} \tag{11}$$

where

$$A = \frac{1}{4} + \varepsilon + \varsigma_0, B = -(2\varepsilon+\varsigma_0-\varsigma_1), C = \varepsilon - \varsigma_1 + \gamma\}. \tag{12}$$

To find the constant k, the discriminant of the expression under the square root of Eq. (11) must be equal to zero. As such, we have:

$$k = \varsigma_0 + \varsigma_1 - 2\gamma \pm 2\sqrt{\varepsilon-\varsigma_1+\gamma}\sqrt{\gamma+\frac{1}{4}}. \tag{13}$$

Substituting Eq. (13) into Eq. (11), we obtain:

$$\pi(x) = -\frac{x}{2} \pm \left(\sqrt{\varepsilon-\varsigma_1+\gamma} + \sqrt{\gamma+\frac{1}{4}}\right)x - \sqrt{\varepsilon-\varsigma_1+\gamma}, \tag{14}$$

with $\tau(x)$ being obtained as:

$$\tau(x) = 1 - 2x - 2\sqrt{\varepsilon-\varsigma_1+\gamma}x - 2\sqrt{\gamma+\frac{1}{4}}x + 2\sqrt{\varepsilon-\varsigma_1+\gamma}. \tag{15}$$

Taking the derivative of Eq. (15) with respect to x, we have:

$$\tau'(x) = -2 - 2\left(\sqrt{\varepsilon-\varsigma_1+\gamma} + \sqrt{\gamma+\frac{1}{4}}\right). \tag{16}$$

Referring to Eq. (A10), we define the constant λ as:

$$\lambda = -\frac{1}{2} - \sqrt{\varepsilon-\varsigma_1+\gamma} - \sqrt{\gamma+\frac{1}{4}} + \varsigma_0 + \varsigma_1 - 2\gamma - 2\sqrt{\varepsilon-\varsigma_1+\gamma}\sqrt{\gamma+\frac{1}{4}}. \tag{17}$$

Also, taking the derivative of $\sigma(x)$ with respect to x from Eq. (10), we have:

$$\sigma''(x) = -2. \tag{18}$$

Substituting Eqs. (15) and (18) into Eq. (A11), we obtain:

$$\lambda_n = n^2 + n + 2n\left(\sqrt{\varepsilon - \varsigma_1 + \gamma} + \sqrt{\gamma + \frac{1}{4}}\right). \quad (19)$$

Equating Eqs. (17) and (19) and substituting Eq.(9) yield the energy eigenvalues equation of the Varshni plus Hellmann potential in the form:

$$E_{nl} = a + \frac{\beta^2\hbar^2 l(l+1)}{2\mu} - \beta c - \frac{\beta^2\hbar^2}{8\mu}\left[\frac{(n+l+1)^2 + \frac{2ab\mu}{\hbar^2\beta} + \frac{2d\mu}{\hbar^2\beta} - \frac{2c\mu}{\hbar^2\beta} + l(l+1)}{(n+l+1)}\right]^2. \quad (20)$$

To obtain the corresponding wave function, we consider Eq. (A4) and upon substituting Eqs. (10) and (14) and integrating, we get:

$$\phi(x) = x^{\sqrt{\varepsilon - \varsigma_1 + \gamma}}(1-x)^{\frac{1}{2}+\sqrt{\frac{1}{4}+\gamma}}. \quad (21)$$

To get the hypergeometric function, we first determine the weight function of Eq. (A6); upon differentiating the left hand side we obtain:

$$\frac{\rho'(x)}{\rho} = \frac{\tau(x) - \sigma'(x)}{\sigma(x)}. \quad (22)$$

Substituting Eqs. (14) and (10) into Eq. (22) and integrating, we simplify obtain:

$$\rho(x) = x^{2\sqrt{\varepsilon - \varsigma_1 + \gamma}}(1-x)^{2\sqrt{\frac{1}{4}+\gamma}}. \quad (23)$$

By substituting Eqs. (10) and (23) into Eq. (A5), we obtain the Rodrigues equation as:

$$y(x) = N_{nl}x^{-2\sqrt{\varepsilon-\varsigma_1+\gamma}}(1-x)^{-2\sqrt{\frac{1}{4}+\gamma}}\frac{d^n}{dx^n}\left[x^{n+2\sqrt{\varepsilon-\varsigma_1+\gamma}}(1-x)^{n+2\sqrt{\frac{1}{4}+\gamma}}\right] \quad (24)$$

where N_{nl} is the normalization constant. Equation (24) is a equivalent to:

$$P_n^{\left(2\sqrt{\varepsilon-\varsigma_1+\gamma},2\sqrt{\frac{1}{4}+\gamma}\right)}(1-2x) \quad (25)$$

where $p_n^{(\alpha,\beta)}$ is the Jacobi Polynomial. The wave function is given as:

$$\psi_{nl}(x) = N_{nl}x^{\sqrt{\varepsilon-\varsigma_1+\gamma}}(1-x)^{\frac{1}{2}+\sqrt{\frac{1}{4}+\gamma}}P_n^{\left(2\sqrt{\varepsilon-\varsigma_1+\gamma},2\sqrt{\frac{1}{4}+\gamma}\right)}(1-2x). \quad (26)$$

Using the normalization condition, we obtain the normalization constant as follows:

$$\int_0^\infty |\psi_{nl}(r)|^2\, dr = 1. \quad (27)$$

From our coordinate transformation of Eq. (7), we have:

$$-\frac{1}{\beta x}\int_1^0 |\psi_{nl}(x)|^2\, dx = 1. \quad (28)$$

By letting $y = 1 - 2x$, we have:

$$\frac{N_{nl}^2}{\beta}\int_{-1}^{1}\left(\frac{1-y}{2}\right)^{2\sqrt{\varepsilon+\gamma}}\left(\frac{1+y}{2}\right)^{1+2\sqrt{\frac{1}{4}+\gamma}}\left[P_n^{\left(2\sqrt{\varepsilon+\gamma},2\sqrt{\frac{1}{4}+\gamma}\right)}y\right]^2 dy = 1. \quad (29)$$

Let

$$\left.\upsilon = 1 + 2\sqrt{\frac{1}{4}+\gamma},\ \upsilon - 1 = 2\sqrt{\frac{1}{4}+\gamma},\ u = 2\sqrt{\varepsilon+\gamma}\right\}. \quad (30)$$

By substituting Eq. (30) into Eq. (29), we have:

$$\frac{N_{nl}^2}{\beta}\int_{-1}^{1}\left(\frac{1-y}{2}\right)^u\left(\frac{1+y}{2}\right)^\upsilon\left[P_n^{(2u,\upsilon-1)}y\right]^2 dy = 1. \quad (31)$$

According to Onate and Ojonubah [53], the integral of the form in Eq. (31) can be expressed as:

$$\int_{-1}^{1}\left(\frac{1-p}{2}\right)^x\left(\frac{1+p}{2}\right)^y\left[P_n^{(2x,2y-1)}p\right]^2 dp = \frac{2\Gamma(x+n+1)\Gamma(y+n+1)}{n!x\Gamma(x+y+n+1)}. \quad (32)$$

Hence, by comparing Eq. (31) with the standard integral of Eq. (32), we obtain the normalization constant as:

$$N_{nl} = \sqrt{\frac{n!u\beta\,\Gamma(u+\upsilon+n+1)}{2\Gamma(u+n+1)\Gamma(\upsilon+n+1)}}. \quad (33)$$

3. Results and Discussion

In this section, we present the numerical results of the energy eigenvalues in atomic mass units $(\hbar = 2\mu = 1)$ of VHP as a function of the screening parameter for 1S, 2S, 2P, 3S, 3P, 3d, 4S and 4P states with three different values of the potential range: $a = -1, b = 1, c = 1, d = -1$; $a = -2, b = 2, c = 2, d = -2$ and $a = 1$, $b = -1$, $c = 4$, $d = -4$, respectively, as presented in Table 1. It is observed that as the potential range increases, the energy of the system decreases. It is also observed that as the orbital angular momentum quantum number increases, the energy of the system increases. We then apply the spectroscopic data obtained from Ref. [54], as presented in Table 2, to compute the ro-vibrational energies of VHP for the diatomic molecules of LiH, TiH, CrH and ScN with the help of Eq. (20) and the numerical computation is presented in Table 3. Here, we have implemented the conversions: $1\ \text{amu} = 931.494028\,\text{MeV}/c^2$ and $\hbar c = 1973.29\ \text{eV}\mathring{\text{A}}$ [55]. It is observed that for each vibrational quantum number, the ro-vibrational energy increases with the increase in the rotational quantum number, for each selected diatomic molecule.

TABLE 1. Energy eigenvalues (eV) of the VHP in atomic mass units $(\hbar = 2\mu = 1)$.

State	α	$a = -1, b = 1,$ $c = 1, d = -1$	$a = -2, b = 2,$ $c = 2, d = -2$	$a = 1, b = -1,$ $c = 4, d = -4$
1s	0.025	-3.237656250	-17.95015625	-19.23765625
	0.050	-3.225625000	-17.90062500	-19.22562500
	0.075	-3.213906249	-17.85140626	-19.21390625
	0.100	-3.202500000	-17.80250000	-19.20250000
	0.150	-3.180625000	-17.70562499	-19.18062500
2s	0.025	-1.550625000	-5.950625000	-4.050625000
	0.050	-1.540000000	-5.902500000	-4.040000000
	0.075	-1.530625000	-5.855625002	-4.030625000
	0.100	-1.522500000	-5.810000000	-4.022500000
	0.150	-1.510000000	-5.722499998	-4.010000000
2p	0.025	-1.540351562	-5.924726562	-4.021601562
	0.050	-1.517656250	-5.848906250	-3.980156250
	0.075	-1.494414062	-5.772539065	-3.938164062
	0.100	-1.470625000	-5.695625000	-3.895625000
	0.150	-1.421406250	-5.540156250	-3.808906250
3s	0.025	-1.238906250	-3.729184028	-1.238906250
	0.050	-1.230625000	-3.683402778	-1.230625000
	0.075	-1.225156250	-3.640434028	-1.225156250
	0.100	-1.222500000	-3.600277778	-1.222500000
	0.150	-1.225625000	-3.528402777	-1.225625000
3p	0.025	-1.233819444	-3.717152778	-1.225486111
	0.050	-1.218611111	-3.657500000	-1.201944445
	0.075	-1.204375000	-3.598819444	-1.179375000
	0.100	-1.191111111	-3.541111111	-1.157777778
	0.150	-1.167500000	-3.428611110	-1.117500000
3d	0.025	-1.227517361	-3.703906250	-1.210850695
	0.050	-1.227517361	-3.626736111	-1.168402778
	0.075	-1.172656250	-3.546267361	-1.122656250
	0.100	-1.140277778	-3.462500000	-1.073611111
	0.150	-1.065625000	-3.285069444	-0.9656250000
4s	0.025	-1.130625000	-2.952500000	-0.2556250000
	0.050	-1.125625000	-2.910000000	-0.2506250000
	0.075	-1.125625000	-2.872500000	-0.2506250000
	0.100	-1.130625000	-2.840000000	-0.2556250000
	0.150	-1.155625000	-2.790000000	-0.2806249998
4p	0.025	-1.127353516	-2.945322266	-0.2476660160
	0.050	-1.117226562	-2.893789062	-0.2328515620
	0.075	-1.110244141	-2.845400390	-0.2211816405
	0.100	-1.106406250	-2.800156250	-0.2126562500
	0.150	-1.108164062	-2.719101562	-0.2050390622

TABLE 2. Model parameters for some selected diatomic molecules in this study [57].

Molecule	$\mu(amu)$	$\alpha\left(\overset{0}{\mathrm{A}}{}^{-1}\right)$
LiH	0.880122100	1.12800
TiH	0.987371000	1.32408
CrH	0.988976000	1.52179
ScN	10.68277100	1.50680

TABLE 3. Energy spectra (in eV) of Varshni plus Hellmann potential for various n and l quantum numbers of LiH, TiH, CrH and ScN diatomic molecules.

n	l	LiH	TiH	CrH	ScN
0	0	-3.256755417	-3.649087811	-4.044803588	-4.013711055
1	0	-3.259021670	-3.651871246	-4.048474354	-4.014044221
1	1	-3.258350187	-3.651046525	-4.047386719	-4.013945505
2	0	-3.262798757	-3.656510305	-4.054592298	-4.014599497
2	1	-3.263601388	-3.657496105	-4.055892360	-4.014717493
2	2	-3.259897954	-3.652947508	-4.049893716	-4.014173045
3	0	-3.268086680	-3.663004987	-4.063157419	-4.015376884
3	1	-3.270383149	-3.665825534	-4.066877128	-4.015714492
3	2	-3.268170615	-3.663108077	-4.063293372	-4.015389223
3	3	-3.261426672	-3.654825096	-4.052369861	-4.014397784
4	0	-3.274885437	-3.671355293	-4.074169717	-4.016376381
4	1	-3.278683508	-3.676020123	-4.080321649	-4.016934742
4	2	-3.277968774	-3.675142279	-4.079163956	-4.016829668
4	3	-3.272725415	-3.668702331	-4.070671018	-4.016058832
4	4	-3.248634679	-3.656693577	-4.054833994	-4.014621434
5	0	-3.283195030	-3.681561221	-4.087629193	-4.017597989
5	1	-3.288498369	-3.688074838	-4.096219285	-4.018377642
5	2	-3.289285583	-3.689041704	-4.097494377	-4.018493372
5	3	-3.285545217	-3.684447747	-4.091435914	-4.017943494
5	4	-3.277272556	-3.674287178	-4.078036258	-4.016727315
5	5	-3.264465670	-3.658557625	-4.057292283	-4.014844553

We have presented the plot of energy spectra of VHP as a function of vibrational quantum number in the ground state in Figs. 2-5. It is observed that there is a decrease in energy in the ground state as the vibrational and rotational quantum numbers increase. In Figs. 6 and 7, we plotted the energy spectra of VHP *versus* the potential strengths a, c. Here, the energy decreases as the potential strengths increase.

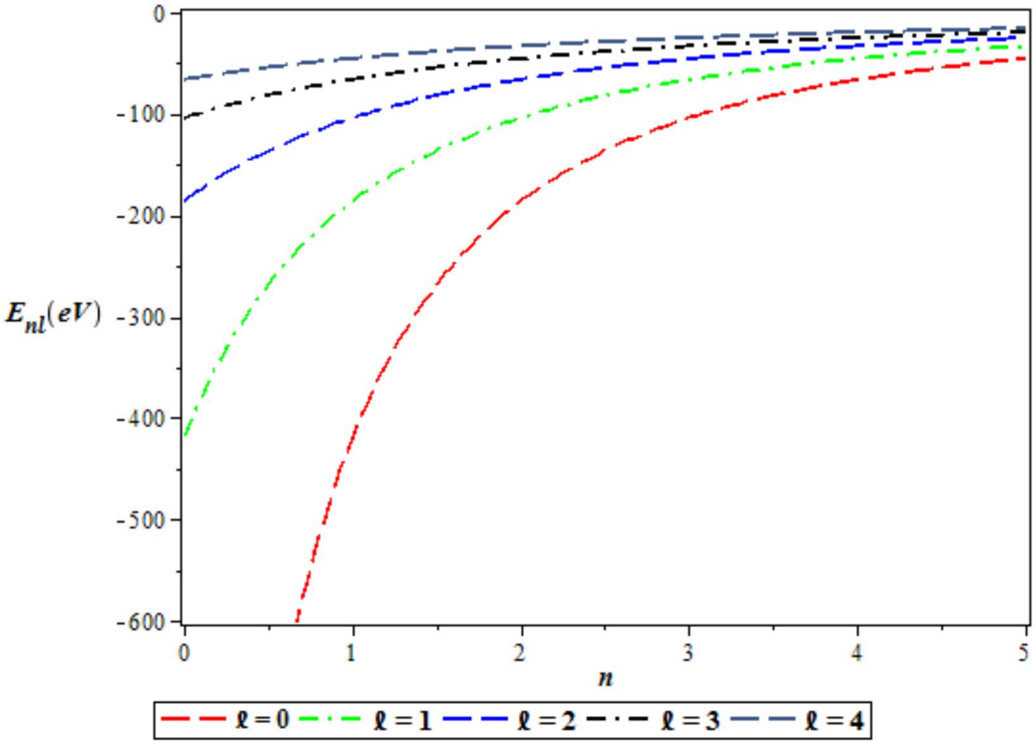

FIG. 2. Variation of the ground-state energy spectra of LiH molecule for various l as a function of n. We choose $a = 1, b = -1, c = 2\ and\ d = -1$·

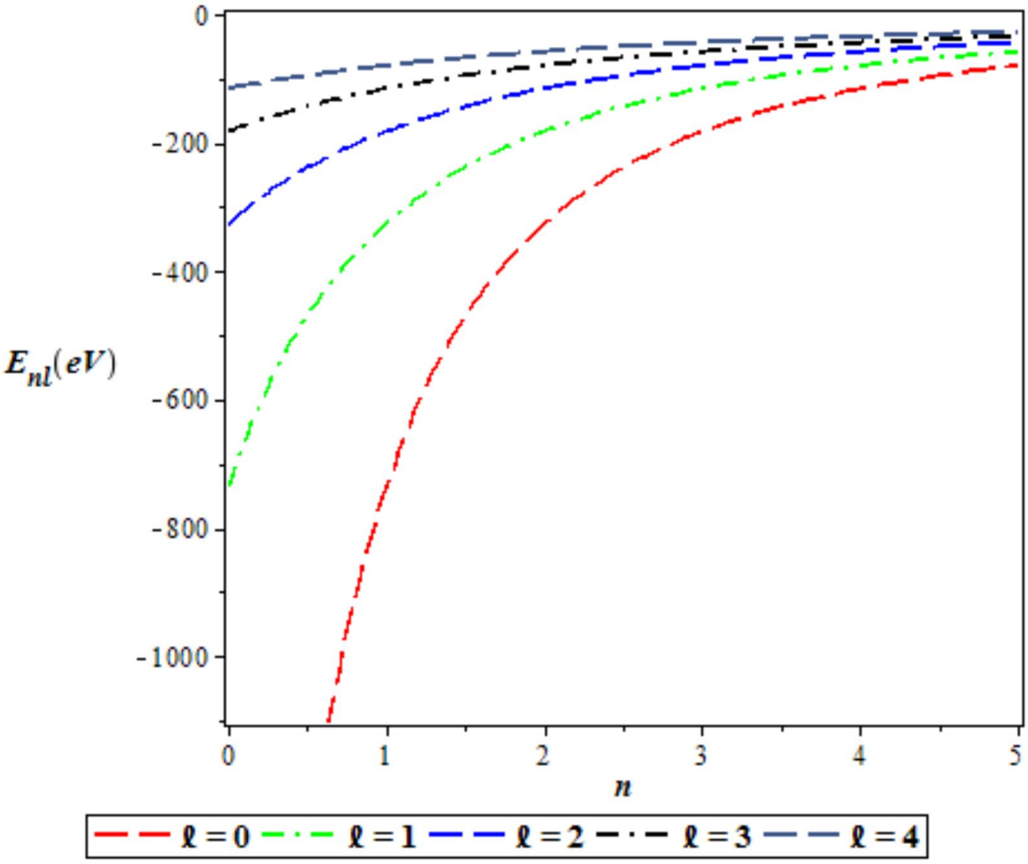

FIG. 3. Variation of the ground-state energy spectra of TiH molecule for various l as a function of n .We choose $a = 1, b = -1, c = 2\ and\ d = -1$·

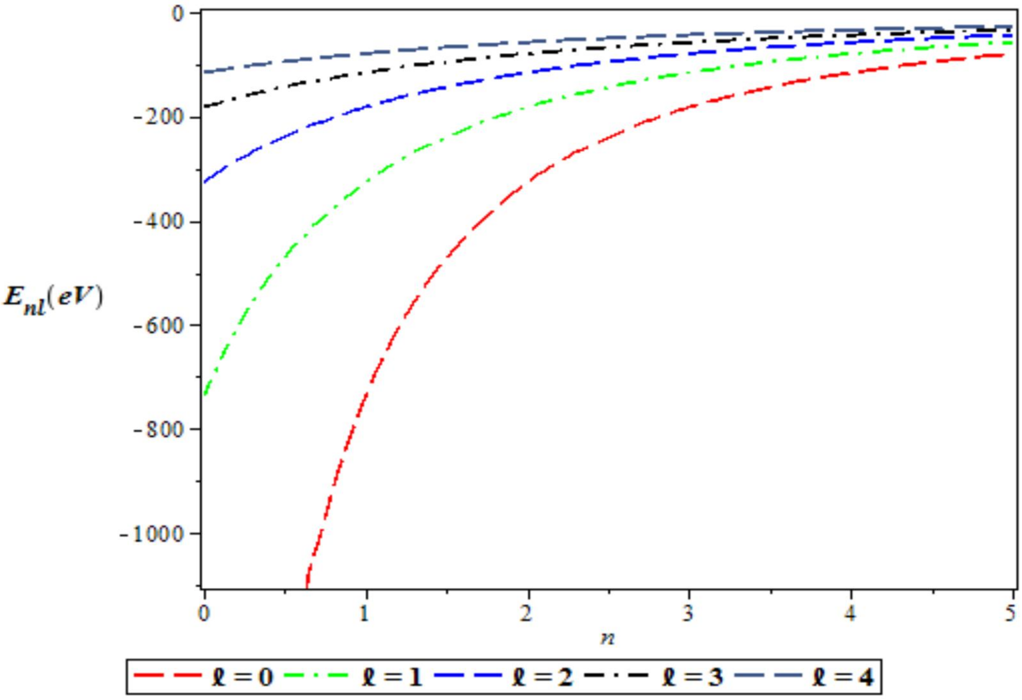

FIG. 4. Variation of the ground-state energy spectra of CrH molecule for various l as a function of n .We choose $a = 1, b = -1, c = 2$ and $d = -1$·

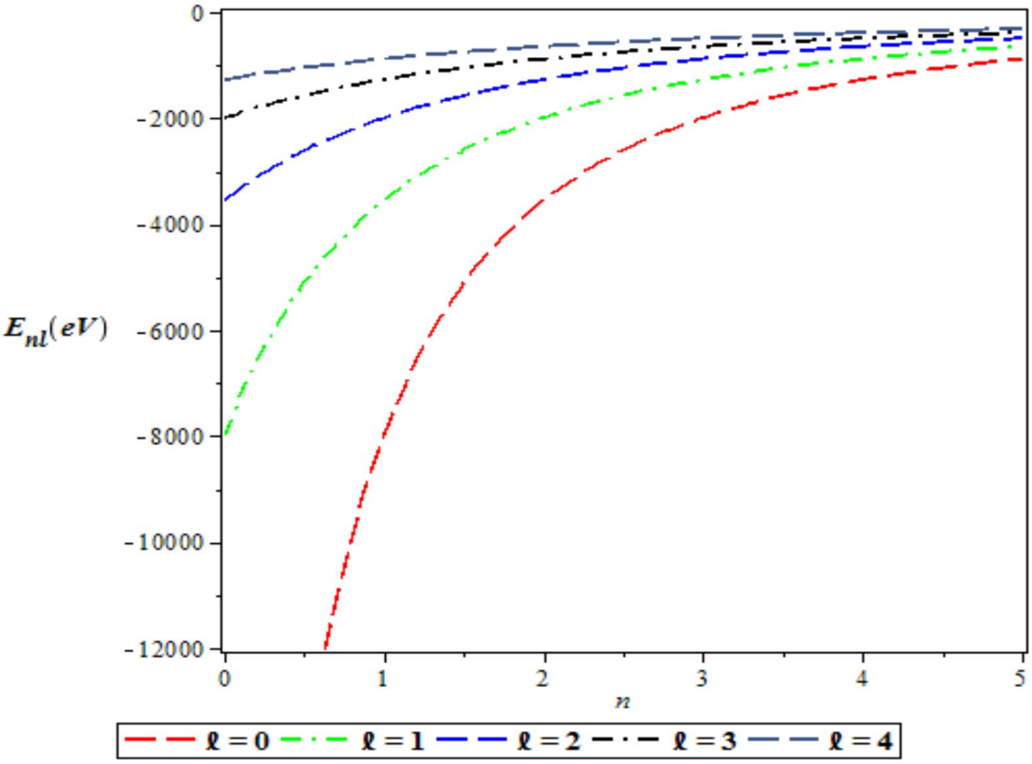

FIG. 5. Variation of the ground-state energy spectra of ScN molecule for various l as a function of n .We choose $a = 1, b = -1, c = 2$ and $d = -1$·

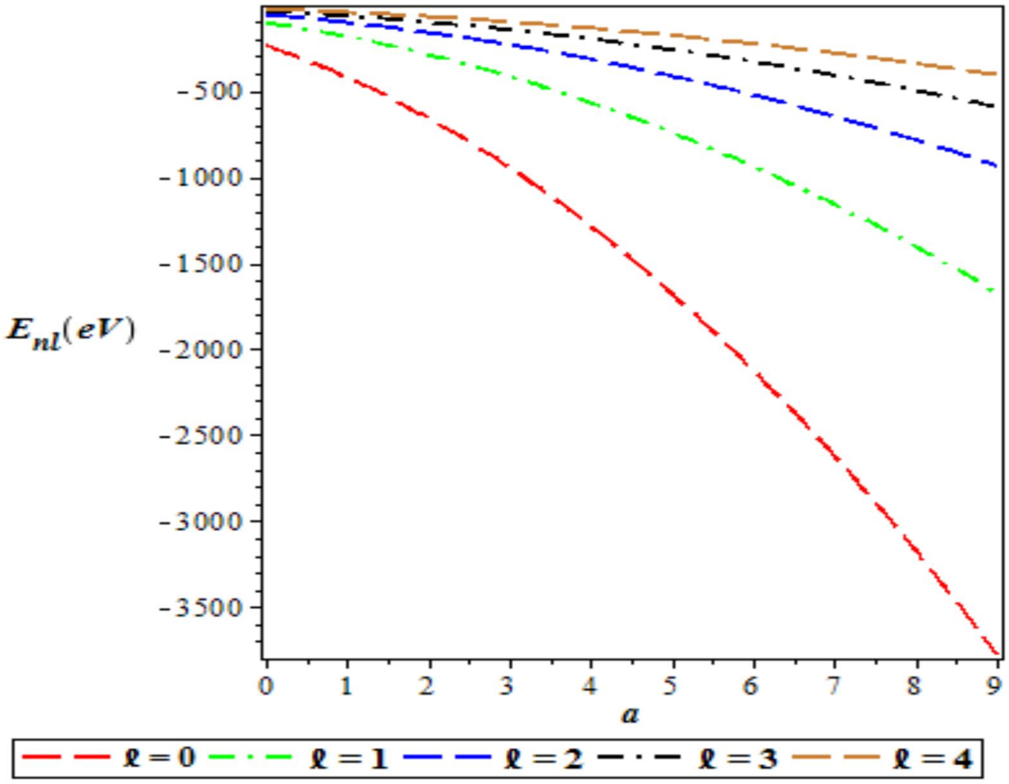

FIG. 6. Variation of the ground-state energy spectra of LiH molecule for various l as a function of a .We choose $a = 1, b = -1, c = 2\ and\ d = -1$·

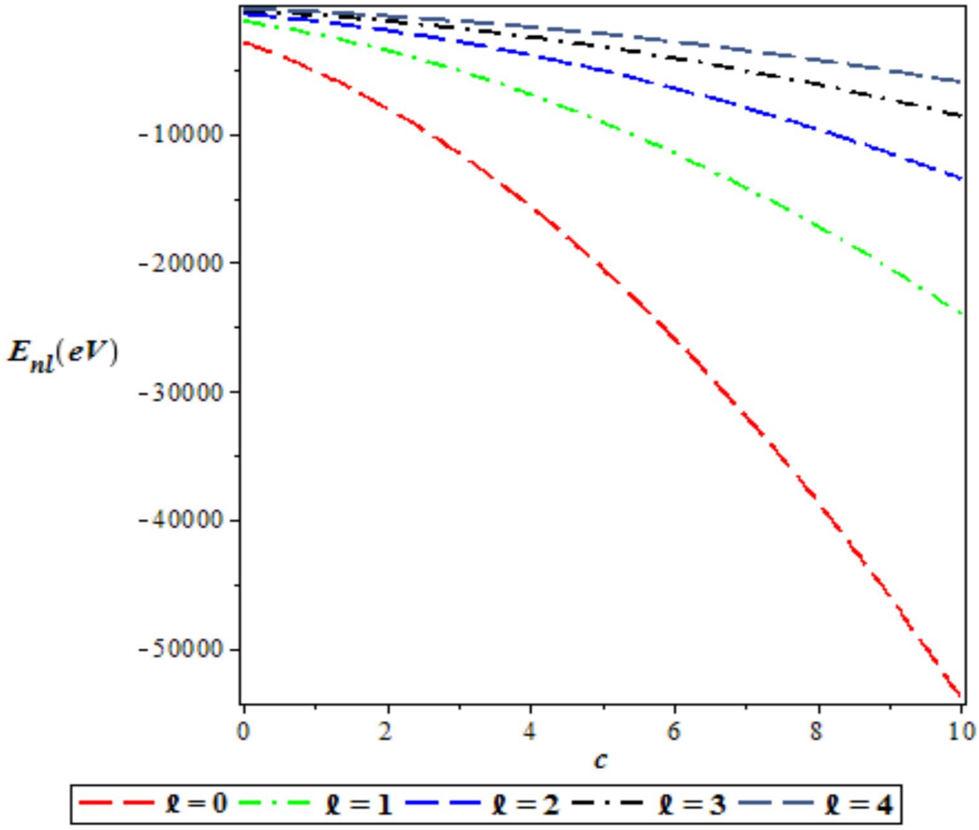

FIG. 7. Variation of the ground-state energy spectra of ScN molecule for various l as a function of c .We choose $a = 1, b = -1, c = 2\ and\ d = -1$·

Special Cases

In this sub-section, we present the energy eigenvalues for adjusted VHP as special cases in order to test for the accuracy of our results.

1) By setting the Varshni potential strength to zero in Eq. (20); i.e., $a = b = 0$, we obtain the energy eigenvalue equation for Hellmann potential as:

$$E_{nl} = \frac{\beta^2\hbar^2 l(l+1)}{2\mu} - \beta c - \frac{\beta^2\hbar^2}{8\mu}\left[\frac{(n+l+1)^2 + \frac{2\mu}{\hbar^2\beta}(d-c) + l(l+1)}{(n+l+1)}\right]^2. \qquad (34)$$

Eq. (34) is in agreement with Eq. (38) of Ref. [21]. The numerical energy eigenvalues are presented in Table 4 for $c = 2$ and $d = -1$. The results are in good agreement with the earlier results of [21] with NU and AP, as well as the PT method of [56].

TABLE 4. Energy eigenvalues (eV) in atomic mass units $(\hbar = 2\mu = 1)$ of Hellmann potential as a function of the screening parameter α for $a = b = 0, c = 2$ and $d = -1$.

State	α	Present method	(NU) [52]	(AP) [52]	(PT) [53]
1S	0.001	−2.250500250	-2.250 500	- 2.248 981	- 2.249 000
	0.005	−2.252506250	-2.252 506	- 2.244 993	- 2.245 010
	0.01	−2.255025000	-2.255 025	- 2.240 030	- 2.240 050
2S	0.001	−0.5630010000	- 0.563 001	- 0.561 502	- 0.561 502
	0.005	−0.5650250000	- 0.565 025	- 0.557 549	- 0.557 550
	0.01	−0.5676000000	- 0.567 600	- 0.552 697	- 0.552 697
2P	0.001	−0.5622502500	- 0.563 000	- 0.561 502	- 0.561 502
	0.005	−0.5612562500	- 0.565 000	- 0.557 541	- 0.557 541
	0.01	−0.5600250000	- 0.567 500	- 0.552 664	-0.552 664
3S	0.001	−0.2505022500	- 0.250 502	- 0.249 004	- 0.249 004
	0.005	−0.2525562500	- 0.252 556	-0245 110	- 0.245 111
	0.01	−0.2552250000	- 0.255 225	-0.240 435	- 0.240 435
3p	0.001	−0.2501680278	-0.250 501	- 0.249 004	- 0.249 004
	0.005	−0.2508673611	-0.252 531	-0.245 102	-0.245 103
	0.01	−0.2518027778	-0.255 125	-0.240 404	-0:240 404
3d	0.001	−0.2495002500	-0.250 833	-0.249 003	-0.249 003
	0.005	−0.2475062500	-0.254 151	-0.245 086	-0.245 086
	0.01	−0.2450250000	-0.258 269	-0.240 341	-0.240 341
4S	0.001	−0.1411290000	-0.141 129	-0.139 633	-0.139 633
	0.005	−0.1432250000	-0.143 225	-0.135 819	-0.135 819
	0.01	−0.1460250000	-0.146 025	-0.131 380	-0.131 381
4p	0.001	−0.1409405625	-0.141 128	-0.139 632	0.139 633
	0.005	−0.1422640625	-0.143 200	-0.135 811	0.135 811
	0.01	−0.1440562500	-0.145 925	-0.131 350	-0.131 351
4d	0.001	−0.1405640625	-0.141 314	-0.139 632	-0.139 632
	0.005	−0.1403515625	-0.144 089	-0.135 795	-0.135 796
	0.01	−0.1401562500	-0.147 606	-0.131 290	-0.131 290
4f	0.001	−0.1400002500	-0.141 686	-0.139 631	-0.139 631
	0.005	−0.1375062500	-0.145 902	-0.135 772	-0.135 772
	0.01	−0.1344000000	-0.151 106	-0.131 200	-0.131 200

2) If we set the Hellmann potential strength to zero in Eq. (20); i.e., $c = d = 0$, we obtain the energy eigenvalue equation for Varshni potential as:

$$E_{nl} = a + \frac{\beta^2\hbar^2 l(l+1)}{2\mu} - \frac{\beta^2\hbar^2}{8\mu}\left[\frac{(n+l+1)^2 + \frac{2ab\mu}{\hbar^2\beta} + l(l+1)}{(n+l+1)}\right]^2. \qquad (35)$$

The numerical energy eigenvalues are presented in Table 5 for three ranges of Varshni potential strength. It is observed that as the screening parameter increases, the energy of the system decreases. Similarly, by interchanging Varshni potential strength, the energy increases in the same proportion as the screening parameter increases. In order to test the accuracy of our results, we compared the result of Varshni potential with the result of Ebomwonyi et al. [49] who used the formula method. As can be seen from Table 5, our result is in agreement with previous results.

3) If we set $a = b = c = 0$ in Eq. (20), we obtain the energy eigenvalues for Yukawa potential as:

$$E_{nl} = \frac{\beta^2\hbar^2 l(l+1)}{2\mu} - \frac{\beta^2\hbar^2}{8\mu}\left[\frac{(n+l+1)^2 + \frac{2d\mu}{\hbar^2\beta} + l(l+1)}{(n+l+1)}\right]^2 . \tag{36}$$

It is observed that as the screening parameter increases, the energy eigenvalue increases. The results are in good agreement with the earlier results of [57] with AIM and [58] of the numerical method.

TABLE 5. Energy eigenvalues (eV) in atomic mass units $(\hbar = 2\mu = 1)$ of Varshni potential as a function of the screening parameter α .

State	α	Present method $a = b = -1$	(FM) [48] $a = b = -1$	Present method $a = -1, b = -2$	Present method $a = -2, b = -1$
1S	0.001	−1.063124562	-	−2.001000250	−3.001000250
	0.050	−1.092656250	-	−2.050625000	−3.050625000
	0.100	−1.120625000	-	−2.102500000	−3.102500000
2S	0.001	−1.063001000	-	−1.251001000	−2.251001000
	0.050	−1.090000000	-	−1.302500000	−2.302500000
	0.100	−1.122500000	-	−1.360000000	−2.360000000
2P	0.001	−1.063124562	-1.0617502	−1.251249562	−2.251249562
	0.050	−1.092656250	-1.0256250	−1.311406250	−2.311406250
	0.100	−1.120625000	-0.9900000	−1.370625000	−2.370625000
3S	0.001	−1.028280028	-	−1.112113361	−2.112113361
	0.050	−1.058402778	-	−1.166736111	−2.166736111
	0.100	−1.100277778	-	−1.233611111	−2.233611111
3p	0.001	−1.028334111	-	−1.112223000	−2.112223000
	0.050	−1.057500000	-	−1.168611111	−2.168611111
	0.100	−1.091111111	-	−1.230000000	−2.230000000
3d	0.001	−1.028386250	- 1.0269447	−1.112330694	−2.112330694
	0.050	−1.051736111	- 0.9867361	−1.165625000	−2.165625000
	0.100	−1.062500000	- 0.9469444	−1.206944444	−2.206944444
4S	0.001	−1.016129000	-	−1.063504000	−2.063504000
	0.050	−1.050625000	-	−1.122500000	−2.122500000
	0.100	−1.105625000	-	−1.202500000	−2.202500000
4p	0.001	−1.016158766	- 1.0150656	−1.063565016	−2.063565016
	0.050	−1.048476562	- 0.9951563	−1.121914062	−2.121914062
	0.100	−1.093906250	- 0.9900000	−1.193906250	−2.193906250
4d	0.001	−1.028386250	- 1.0149391	−1.063624062	−2.063624062
	0.050	−1.051736111	- 0.9851563	−1.116406250	−2.116406250
	0.100	−1.062500000	- 0.9625000	−1.063624062	−2.165625000
4f	0.001	−1.016212391	- 1.0147502	−1.063681141	−2.063681141
	0.050	−1.029414062	- 0.9725000	−1.105976562	−2.105976562
	0.100	−1.011406250	- 0.9306250	−1.117656250	−2.117656250

4) If we set $a = b = d = \beta = 0$ in Eq. (20), we obtain the energy eigenvalues for Coulomb potential as:

$$E_{nl} = -\frac{\mu c^2}{2\hbar^2 (n+l+1)^2} . \tag{37}$$

The result of Eq. (37) is consistent with the result obtained by Eq. (36) in Ref. [47].

TABLE 6. Energy eigenvalues (eV) in atomic mass units $(\hbar = \mu = 1)$ of Yukawa potential as a function of the screening parameter α with $d = \sqrt{2}$.

State	α	Present method	AIM[54]	Numerical[55]	SUSY[56]
1S	0.002	- 0.9954605000	−0.99600	−0.99600	−0.99601
	0.005	- 0.9835031250	−0.99003	−0.99004	−0.99000
	0.010	−0.980100000	−0.98014	−0.98015	−0.98010
	0.020	−0.960400000	−0.96059	−0.96059	−0.96060
	0.025	−0.950620000	−0.95092	−0.95092	−0.95090
	0.050	−0.90250000	−0.90363	−0.90363	−0.90360
2S	0.002	−0.24601000	−0.24602	−0.24602	−0.24600
	0.005	−0.24010000	−0.24014	−0.24015	−0.24010
	0.010	−0.23040000	−0.23058	−0.23059	−0.20360
	0.020	−0.21160000	−0.21229	−0.21230	−0.21230
	0.025	−0.20250000	−0.20355	−0.20355	−0.23060
	0.050	−0.16000000	−0.16354	−0.16351	−0.16350
2P	0.002	−0.24601000	−0.24601	−0.24602	−0.24600
	0.005	−0.24010000	−0.24012	−0.24012	−0.24010
	0.010	−0.23040000	−0.23049	−0.23049	−0.23050
	0.020	−0.21160000	−0.21192	−0.21192	−0.21190
	0.025	−0.20250000	−0.20298	−0.20299	−0.20300
	0.050	−0.16000000	−0.16148	−0.16144	−0.16150
3p	0.002	−0.10714000	−0.10716	−0.10716	−0.10720
	0.005	−0.10133000	−0.10141	−0.10142	−0.10140
	0.010	−0.09201000	−0.09230	−0.09231	−0.09231
	0.020	−0.07471000	−0.07570	−0.07570	−0.07570
	0.025	−0.06673000	−0.06815	−0.06814	−0.06816
	0.050	−0.03361000	−0.03711	−0.03739	−0.03712
3d	0.002	−0.10714000	−0.10715	−0.10715	−0.10720
	0.005	−0.10133000	−0.10136	−0.10140	−0.10140
	0.010	−0.09201000	−0.09212	−0.09212	−0.09212
	0.020	−0.07471000	−0.07503	−0.07502	−0.07503
	0.025	−0.06673000	−0.06714	−0.06713	−0.06715
	0.050	−0.03361000	−0.03383	−0.03388	−0.03383

4. Conclusion

In this study, the radial Schrödinger equation for the newly proposed Varshni-Hellmann potential (VHP) is obtained within the framework of the Nikiforov-Uvarov method by employing the Greene-Aldrich approximation scheme to the centrifugal term. The numerical results obtained of the ro-vibrational energies for LiH, TiH, CrH and ScN diatomic molecules are observed to increase with an increase in the quantum state considered. It is noticed that the selected molecular diatomic molecules studied in this work have similar behaviors. By adjusting the potential strength, we deduced four special cases with their numerical energy eigenvalues. The results obtained are in agreement with those of the works of other researchers using different methods. Also, we have discussed the results of the ground-state energy spectra obtained graphically.

Appendix: Review of Nikiforov-Uvarov (NU) Method

The NU method according to Nikiforov and Uvarov is used to transform Schrödinger-like equations into a second-order differential equation through a coordinate transformation $x = x(r)$ of the form [57, 58]:

$$\psi''(x) + \frac{\tilde{\tau}(x)}{\sigma(x)}\psi'(x) + \frac{\tilde{\sigma}(x)}{\sigma^2(x)}\psi(x) = 0 \quad \text{(A1)}$$

where $\tilde{\sigma}(x)$ and $\sigma(x)$ are polynomials, at most second-degree, while $\tilde{\tau}(x)$ is a first-degree polynomial.

The exact solution of Eq. (A1) can be obtained by using the transformation:

$$\psi(x) = \phi(x) y(x). \tag{A2}$$

This transformation reduces Eq.(A1) into a hypergeometric-type equation of the form:

$$\sigma(x) y''(x) + \tau(x) y'(x) + \lambda y(x) = 0\ . \tag{A3}$$

The function $\phi(x)$ can be defined as the logarithm derivative:

$$\frac{\phi'(x)}{\phi(x)} = \frac{\pi(x)}{\sigma(x)}, \tag{A4}$$

with $\pi(x)$ being at most a first-degree polynomial. The second part of the wave function in Eq. (A2) is a hypergeometric-type function obtained by Rodrigues relation:

$$y(x) = \frac{N_{nl}}{\rho(x)} \frac{d^n}{dx^n}\left[\sigma^n(x)\rho(x)\right] \tag{A5}$$

where N_{nl} is the normalization constant and $\rho(x)$ the weight function which satisfies the condition below;

$$\left(\sigma(x)\rho(x)\right)' = \tau(x)\rho(x) \tag{A6}$$

where also

$$\tau(x) = \tilde{\tau}(x) + 2\pi(x). \tag{A7}$$

For bound solutions, it is required that:

$$\frac{d\tau(x)}{dx} < 0\ . \tag{A8}$$

The eigenfunctions and eigenvalues can be obtained using the definition of the following function $\pi(x)$ and parameter λ, respectively:

$$\pi(x) = \frac{\sigma'(x) - \tilde{\tau}(x)}{2} \pm \sqrt{\left(\frac{\sigma'(x) - \tilde{\tau}(x)}{2}\right)^2 - \tilde{\sigma}(x) + k\sigma(x)} \tag{A9}$$

and

$$\lambda = k_- + \pi'_-(x). \tag{A10}$$

The value of k can be obtained by setting the discriminant in the square root in Eq. (A9) equal to zero. As such, the new eigenvalue equation can be given as

$$\lambda_n + n\tau'(x) + \frac{n(n-1)}{2}\sigma''(x) = 0, (n = 0,1,2,\ldots). \tag{A11}$$

References

[1] Inyang, E.P., William, E.S. and Obu, J.A., Rev. Mex. Fis., 67 (2021) 193.

[2] Inyang, E.P., Inyang, E.P., Ntibi, J.E. and William, E.S., Bulletin of Pure & Applied Sciences- Physics, 40d (2021) 14.

[3] Alsadi, K.S., J. Taibah Uni. Sci., 14 (2020) 1163.

[4] Inyang,E.P.,William,E.S., Obu,J.O., Ita,B.I., Inyang,E.P.,and Akpan,1.O., Mol. Phys., 119 (2021) e1956615. https://doi.org/10.1080/00268976.2021.1956615

[5] Inyang,E.P., Inyang, E.P., Akpan, I.O., Ntibi, J.E. and William, E.S., Can. J. Phys., 99 (2021) 990.https://doi.org/10.1139/cjp-2020-0578.

[6] Ibekwe, E.E., Okorie, U.S., Emah, J.B., Inyang, E.P. and Ekong, S.A., Eur. Phys. J. Plus, 87 (2021) 136.

[7] Inyang, E.P., Inyang, E.P., William, E.S. and Ibekwe, E.E., Jordan J. Phys., 14 (4) (2021) 337.

[8] Inyang, E.P., William, E.S., Omugbe, E., Inyang, E.P., Ibanga, E.A., Ayedun, F., Akpan, I.O. and Ntibi, J.E., Rev. Mex. Fis., 68 (2022) 14.

[9] Inyang, E.P., Ntibi, J.E., Inyang, E.P., William, E.S. and Ekechukwu, C.C., Intl. Innov. Sci. Engr. Tech., **7** (2020)

[10] Inyang, E.P., Inyang, E.P., Ntibi, J.E., Ibekwe. E.E. and William, E.S., Ind. J. Phys., 95 (2021) 2733.

[11] Romaniega, C., Gadella, M., Betan, R.M. *et al.,* Eur. Phys. J. Plus, 135 (2020) 372.

[12] Zhang, M.C., Chin. Phys. Lett., 30 (2013) 11030.

[13] Zhang, L.H., Li, X.P. and Jia, C.S., Intl. J. Quan. Chem., 111 (2011) 870.

[14] Makarov, A.A., Smorodinsky, J.A., Valiev, K.H. and Winternitz, P., Nuov. Cim. A, 52 (1967) 1061.

[15] Ahmadov, H.I., Jafarzade, S.I. and Qocayeva, M.V., Int. J. Mod. Phys. A, 30 (2015) 1550193.

[16] Inyang, E.P., Iwuji, P.C., Ntibi, J.E., William, E.S. and Ibanga, E.A. East Eur. J. Phys.1(2022)11.https://doi.org/10.26565/2312-4334-2022-2-02

[17] Pekeris, C.L., Phys. Rev., 45 (1934) 98.

[18] Greene, R.L. and Aldrich, C., Phys. Rev. A, 14 (1976) 2363.

[19] Inyang, E.P., William, E.S. and Obu, J.A., Revista Mexicana de Física, 67 (2) (2021) 193.

[20] Omugbe, E., Osafile, O.E., Okon,,I. B., Eyube ,E.S., Inyang, E.P., Okorie U.S., Jahanshir, A. and Onate,C.A., Eur. Phys. J. D.,76:72 (2022)11.

[21] William, E.S., Inyang, E.P. and Thompson, E.A., Rev. Mex. Fis., 66 (2020) 730.

[22] Ahmadov, A., Demirci, M., Aslanova, S. and Mustamin, M., Phys. Lett. A, 384 (2020) 126372.

[23] Ahmadov, A., Aydin, C. and Uzun, O., Int. J. Mod. Phys. A, 29 (2014) 1450002.

[24] Aspoukeh, P. and Hamad, S.M., Chin. J. Phys., 68 (2020) 235.

[25] Hellmann, H., J. Chem. Phys., 3 (1935) 61.

[26] Callaway, J. and Laghos, P., Phys. Rev., 187 (1969) 192.

[27] William, E.S., Obu, J.A., Akpan, I.O., Thompson, E.A. and Inyang, E.P., European Journal of Applied Physics, 2 (6) (2020) 28.

[28] Kleinman, L. and Phillips, J.C., Phys. Rev., 116 (1959) 880.

[29] Hughes, A.J. and Callaway, J., Phys. Rev., 136 (1964) A1390.

[30] Akpan, I.O., Inyang, E.P., Inyang, E.P. and William, E.S., Revista Mexicana de Física, 67 (3) (2020) 482.

[31] McGinn, G., J. Chem. Phys., 53 (1970) 3635.

[32] Gryaznov, V.K., Zhernokletov, M.V., Zubarev, V.N., Losilevskii, I.L. and Tortov, V.E., J. Exp. Theo. Phys., 78 (1980) 573.

[32] William, E.S., Inyang, E.P., Akpan, I.O., Obu, J.A., Nwachukwu, A.N. and Inyang, E.P., Indian J. Phys., (2022). https://doi.org/10.1007/s12648-0222-02308-0.

[33] Dutt, R., Mukherji, U. and Varshni, Y.P., Phys. Rev. A, 34 (1986) 777.

[34] Ikhdair, S.M. and Sever, R., Intl. J. Mod. Phys. A, 21 (2006) 6465.

[35] Ntibi, J.E., Inyang, E.P., Inyang, E.P. and William, E.S., Intl. J. Innov. Sci. Engr. Tech., **7** (11) (2020) 28.

[36] Varshni, Y.P. and Shukla, R.C., Rev. Mod. Phys., 35 (1963) 130.

[37] Inyang, E.P., Inyang, E.P., Akpan, I.O., Ntibi, J.E. and William, E.S., European Journal of Applied Physics, 2 (6) (2020) 26

[38] Okoi,P.O., Edet, C.O., Magu, T.O., and Inyang,E.P., Jordan J. Phys. 15(2022)148.

[39] Inyang, E.P., William , E.S., Ntibi, J.E., Obu, J.A., Iwuji, P.C. and Inyang, E.P. Can. J. Phys. (2022). https://doi.org/10.1139/cjp-2022-0030

[40] Omugbe, E., Osafile, O.E., Okon, I.B., Inyang, E.P., William, E.S. and Jahanshir, A., Few-Body Syst., 63 (2022) 7.

[41] Hamzavi, M., Thylwe, K.E. and Rajabi, A.A., Commun. Theo. Phys., 60 (2013) 602.

[42] Roy, A.K., Jalbout, A.F. and Proynow, E.I., arXiv:1307.2983v (2013) [quant-ph].

[43] Onate, C.A., Ojonubah, J.O., Adeoti, A., Eweh, E.J. and Ugboja, M., Afri. Rev. Phys., 9 (2014) 0062.

[44] Arda, A. and Sever, R., Phy. Scripta., 89 (2014) 105204.

[45] Oluwadare, O.J. and Oyewumi, K.J., Adv. High Ener. Phys., 2018 (2018) 5214041.

[46] Edet, C.O., Okorie, U.S., Ngiangia, A.T. and Ikot, A.N., Ind. J. Phys., 37 (2019) 288.

[47] Inyang, E.P., Ntibi, J.E., Ibanga, E.A., Ayedun, F., Inyang, E.P., Ibekwe, E.E., William, E.S. and Akpan, I.O., Comm. Phys. Sci., 7 (2021) 114.

[48] Ebomwonyi, O., Onate, C.A. and Odeyemi, O.E., J. Appl. Sci. Env. Mangt., 23 (2019) 19.

[49] Inyang, E.P., Inyang, E.P., William, E.S., Ibekwe, E.E. and Akpan, I.O., (2020) http://arxiv.org/abs/2012.10639.

[50] William, E.S., Okon, I.B., Ekerenam, O.O., Akpan, I.O., Ita, B.I., Inyang, E.P., Etim, I.P. and Umoh, I.F., Intl. J. Quan. Chem., (2022) e26925.

[51] Hamzavi, M., Thylwe, K.E. and Rajabi, A.A., Commun.Theo. Phys., 60 (2013) 8.

[52] Oluwadere, O.J. and Oyewumi, K.J., Eur. Phys. J. Plus, 133 (2018) 422.

[53] Okon, I.B., Antia, A.D., Akpabio, L.E. and Archibong, B.U., J. Appl. Phys. Sci Intl., 10 (2018) 268.

[54] Ikhdair, S.M and Sever, R., J. Mol. Struct.: THEOCHEM, 809 (2007) 113.

[55] Karakoc, M. and Boztosun, I., Intl. J. Mod. Phys. E, 15 (6) (2006) 1253.

[56] Gonul, B., Koksal, K. and Bakir, E., Phy. Scripta., 98 (2018) 453.

[57] Nikiforov, A.F. and Uvarov, V.B., "Special Functions of Mathematical Physics", (Birkhauser, Basel, 1988) pp. 456-459.

[58] Inyang, E.P., Iwuji, P.C., Ntibi, J.E., Omugbe, E., Ibanga, E.A. and William, E.S., East Eur. J. Phys., 2 (2022) 51.