frontiers | Frontiers in Physics

TYPE Original Research
PUBLISHED 02 September 2022
DOI 10.3389/fphy.2022.988279

OPEN ACCESS

EDITED BY
Akpan Ndem Ikot,
University of Port Harcourt, Nigeria

REVIEWED BY
Reza Khordad,
Yasouj University, Iran
Akaninyene Daniel Antia,
University of Uyo, Nigeria

*CORRESPONDENCE
Uduakobong Sunday Okorie,
uduakobongokorie@aksu.edu.ng

SPECIALTY SECTION
This article was submitted to Atomic and Molecular Physics,
a section of the journal
Frontiers in Physics

RECEIVED 07 July 2022
ACCEPTED 28 July 2022
PUBLISHED 02 September 2022

CITATION
Ibrahim N, Okorie US, Sulaiman N, Rampho GJ and Ramantswana M (2022), Solutions of the Schrodinger equation of the shifted screened Kratzer potential and its thermodynamic functions using the extended Nikiforov–Uvarov method.
Front. Phys. 10:988279.
doi: 10.3389/fphy.2022.988279

Solutions of the Schrodinger equation of the shifted screened Kratzer potential and its thermodynamic functions using the extended Nikiforov–Uvarov method

Nuhu Ibrahim[1], Uduakobong Sunday Okorie[2]*,
Nidhal Sulaiman[3], Gaotsiwe Joel Rampho[4] and
Morris Ramantswana[4]

[1]Department of Physics, University of Maiduguri, Maiduguri, Nigeria, [2]Department of Physics, Akwa Ibom State University, Uyo, Nigeria, [3]Department of Physics, College of Science, Sultan Qaboos University, Muscat, Oman, [4]Department of Physics, University of South Africa, Johannesburg, South Africa

By employing the extended Nikiforov–Uvarov (ENU) method, we solved the radial Schrodinger equation with the shifted screened Kratzer potential model. The analytical expression of the energy eigenvalues and numerical results were determined for some selected diatomic molecule systems. Variations of the energy eigenvalues obtained with potential parameters and quantum numbers were discussed graphically. Also, variations of different thermodynamic properties with temperature and maximum vibration quantum numbers were discussed extensively. Our results correspond to the results obtained in the literatures. The shifting parameters contribute a great effect to the energy results obtained. It has also been established that there exists a critical temperature at specific entropy values for the selected diatomic molecule systems.

KEYWORDS

shifted screened Kratzer potential (SSKP), extended Nikiforov–Uvarov (ENU) method, partition function, entropy, diatomic molecule system

Introduction

Since the inception of quantum mechanics many decades ago, different analytical techniques have been used by different authors to obtain the solutions of the Schrodinger wave equation (SWE), Klein–Gordon equation (KGE), and Dirac equation (DE). Such analytical techniques include the factorization method [1], modified factorization method [2], Nikiforov–Uvarov (NU) method [3], asymptotic iteration method (AIM) [4], Nikiforov–Uvarov functional analysis (NUFA) method [5], and extended Nikiforov–Uvarov (ENU) method [6], among others [7–9]. In recent years, many researchers in quantum mechanics have devoted their interest to finding the solutions of the SWE for different potential models [10–12]. These solutions obtained are either exactly or approximately. In the literature, only a few of these potential models can be solved exactly such as that of a harmonic oscillator and hydrogen atom [13]. It is also well known that the solution obtained from the SWE can be used to study many physical systems such as probability density and information theoretic measures [14–18], thermodynamics properties [19–23], and other applications in physics and chemistry [24–30]. The potential models that have been investigated within the framework of nonrelativistic and relativistic quantum mechanics included the screened Kratzer potential, Hulthen potential, Mobius-square potential, improved screened Kratzer potential, Wood–Saxon potential, Manning–Rosen potential, Yukawa potential, screened Coulomb potential, and others. One of the best potential models used to describe the interaction of a molecular structure in quantum mechanics is the Kratzer potential [31]. The Kratzer potential has many applications in different branches of physics and chemistry such as molecular physics, atomic physics, and quantum chemistry [32]. Recently, Ikot et. al. [33] proposed a screened Kratzer potential and investigated the bound state solution of the SWE with applications to diatomic molecules. In a similar development, Ikot et al. [34] proposed an improved screened Kratzer potential and investigated the bound state solutions of the Klein–Gordon equation with applications to the thermodynamic properties within the nonrelativistic limit. One of the special cases of the improved screened Kratzer is the shifted screened Kratzer potential (SSKP), which is our focal point of concern in this study. This is given in the form:

$$V(r) = -2D_e\left(\frac{a}{r} - \frac{b}{2r^2}\right)\left(2\lambda + \gamma e^{-\alpha r}\right), \tag{1}$$

where D_e is the dissociation energy, $a = r_e,\ b = r_e^2,\quad r_e$ being the equilibrium bond length, α is the screening parameter, and λ and γ are constants called “shifting parameters,” and they can be adjusted as desired. The Kratzer potential and the screened Kratzer potential can be obtained from the shifted screened Kratzer potential by adjusting the shifting parameters appropriately. We aim at unveiling the effects experienced by the diatomic molecule systems to be considered, as a result of the existing shifted parameters in the SSKP model. We are also motivated to study the thermodynamics functions of the SSKP for selected diatomic molecule systems, which has not been studied before to the best of our knowledge.

Solutions of the radial Schrodinger equation with the shifted screened Kratzer potential

The radial Schrodinger equation is given as [35]

$$\frac{d^2\psi(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left[E_{n\ell} - V(r) - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right]\psi(r) = 0, \tag{2}$$

where μ is the reduced mass, E_{nl} is the energy spectrum, $\hbar$ is the reduced Planck’s constant, and n and l are the radial and orbital angular momentum quantum numbers, respectively (also known as the vibration-rotation quantum numbers) [36]. Substituting Eq. 1 into Eq. 2 gives

$$\frac{d^2\psi(r)}{dr^2} + \left[\frac{2\mu E_{n\ell}}{\hbar^2} + \frac{4\mu D_e}{\hbar^2}\left(\frac{a}{r} - \frac{b}{2r^2}\right)\left(2\lambda + \gamma e^{-\alpha r}\right) - \frac{\ell(\ell+1)}{r^2}\right]\psi(r) = 0. \tag{3}$$

We employ the Greene–Aldrich approximation scheme to deal with the centrifugal barrier as [37]

$$\frac{1}{r^2} \approx \frac{\alpha^2}{\left(1 - e^{-\alpha r}\right)^2}\ ,\quad \frac{1}{r} \approx \frac{\alpha}{\left(1 - e^{-\alpha r}\right)}. \tag{4}$$

Substituting Eq. 4 into Eq. 3 and using the coordinate transformation of the form $s = e^{-\alpha r}$, we have

$$\frac{d^2\psi(s)}{ds^2} + \frac{(1-s)}{s(1-s)}\frac{d\psi(s)}{ds} + \frac{1}{s^2(1-s)^2}\left[-\left(\epsilon_n^2 + \sigma_3\right)s^2 + \left(2\epsilon_n^2 + \sigma_3 - \sigma_1 - \sigma_4\right)s - \left(\epsilon_n^2 + \sigma_2 + \sigma_5 - \sigma_1\right)\right]\psi(s) = 0, \tag{5}$$

where

$$\varepsilon_n^2 = -\frac{2\mu E}{\hbar^2\alpha^2};\ \sigma_1 = \frac{8\mu D_e a\lambda}{\hbar^2\alpha};\ \sigma_2 = \frac{4\mu D_e b\lambda}{\hbar^2};\ \sigma_3 = \frac{4\mu D_e a\gamma}{\hbar^2\alpha};$$
$$\sigma_4 = \frac{2\mu D_e b\gamma}{\hbar^2};\ \sigma_5 = \ell(\ell+1). \tag{6}$$

Comparing Eq. 5 and Eq. (A1) of the extended Nikiforov–Uvarov (ENU) [6, 38, 39] method (see the Appendix A section), we have the following polynomials:

$$\tilde{\tau}_e(s) = 1 - s, \tag{7}$$

$$\sigma_e(s) = s(1-s), \tag{8}$$

$$\tilde{\sigma}_e(s) = -\left(\varepsilon_n^2 + \sigma_3\right)s^2 + \left(2\varepsilon_n^2 + \sigma_3 - \sigma_1 - \sigma_4\right)s - \left(\varepsilon_n^2 + \sigma_2 + \sigma_5 - \sigma_1\right). \tag{9}$$

Substituting these polynomials into Eq. (A8), we obtain

$$\pi_e(s) = -\frac{s}{2} \pm \sqrt{-Ps^3 + \left(\frac{1}{4} + \varepsilon_n^2 + \sigma_3 + P - Q\right)s^2 - \left(2\varepsilon_n^2 + \sigma_3 - \sigma_1 - \sigma_4 + Q\right)s + \left(\varepsilon_n^2 + \sigma_2 + \sigma_5 - \sigma_1\right)}. \tag{10}$$

Here, we have employed a linear function $G(s) = Ps + Q$, which makes the function under the square in Eq. 10 to become quadratic $\left(A + Bs + Cs^2\right)^2$. Hence,

$$\pi_e(s) = -\frac{s}{2} \pm \quad \left(A + Bs + Cs^2\right), \tag{11}$$

where the coefficients A, B, C, P, Q are defined as follows:

$$\left.\begin{aligned}
&A = \pm\sqrt{\varepsilon_{nl}^2 + \sigma_2 + \sigma_5 - \sigma_1}\ ;\\
&B = \pm\left(\sqrt{\frac{1}{4} + \sigma_2 + \sigma_4 + \sigma_5} - \sqrt{\varepsilon_{nl}^2 + \sigma_2 + \sigma_5 - \sigma_1}\right);\\
&C = 0\,;\quad P = 0\,;\\
&Q = \pm\left(\sqrt{\varepsilon_{nl}^2 + \sigma_2 + \sigma_5 - \sigma_1}\sqrt{\frac{1}{4} + \sigma_2 + \sigma_4 + \sigma_5}\right) + \sigma_1 - 2\sigma_2 + \sigma_3 - \sigma_4 - 2\sigma_{5.}
\end{aligned}\right] \tag{12}$$

By employing Eq. 12, Eq. 11 becomes

$$\pi_e(s) = -\frac{s}{2} \pm (A + Bs). \tag{13}$$

By substituting Eqs 7, 13 into Eq. (A7) (see the Appendix A section), we have

$$\tau_e(s) = 1 - 2s \pm 2(A + Bs). \tag{14}$$

From the knowledge of the ENU method, we choose the expression $\pi_e(s)_-$ in which the function $\tau_e(s)$ has a negative derivative. Hence, Eqs 13, 14 become

$$\pi_e'(s) = -\frac{1}{2}(1 + B) \tag{15}$$

and

$$\tau_e'(s) = -2(1 + B). \tag{16}$$

Referring to Eq. (A9) and by substituting Eq. 16, we define the constant $h(s)$ as

$$h(s) = Q - \frac{1}{2}(1 + B). \tag{17}$$

By substituting Eqs 6, 12, 16, 17 into Eq. A12, where $\sigma''(s) = -2$, we obtain the energy eigenvalue equation of the shifted screened Kratzer potential as

$$\begin{aligned}
E_{n\ell} = \Lambda + \frac{\hbar^2\alpha^2\ell(\ell+1)}{2\mu}\\
- \frac{\hbar^2\alpha^2}{2\mu}\left[\frac{n+\delta}{2} - \frac{\frac{8\mu D_e a\lambda}{\hbar^2\alpha} - \frac{4\mu D_e a\lambda}{\hbar^2} + \frac{4\mu D_e a\gamma}{\hbar^2\alpha} - \ell(\ell+1)}{2(n+\delta)}\right]^2,
\end{aligned} \tag{18}$$

where,

$$\Lambda = -4\alpha D_e a\lambda + 2\alpha^2 D_e b\lambda \tag{19}$$

and

$$\delta = \frac{1}{2}\left(1 \pm \sqrt{(1+2\ell)^2 + \frac{16\mu D_e a\lambda}{\hbar^2} + \frac{8\mu D_e b\gamma}{\hbar^2}}\right). \tag{20}$$

Thermodynamic properties of the shifted screened Kratzer potential

The partition function is the starting point usually employed in investigating different thermodynamic properties of diatomic molecule systems. The partition function is known to be a function of temperature, which is obtained via the expression [40–42]

$$Z(\beta, N_{\max}) = \sum_{n=0}^{N_{\max}} e^{-\beta E_{nl}},\ \beta = \frac{1}{k_B T}. \tag{21}$$

Here, k_B is the Boltzmann's constant, $N_{\max}$ is the maximum vibration quantum number, T is the absolute temperature, and E_{nl} represents the energy eigenvalues of the SSKP model.

By substituting Eq. 18 into Eq. 21, we obtain

$$Z(\beta, N_{\max}) = \sum_{n=0}^{N_{\max}} e^{-\beta\left[G_1 - H\left(\frac{(n+\delta)}{2} - \frac{G_2}{2(n+\delta)}\right)^2\right]}, \tag{22}$$

where

$$\left.\begin{aligned}
&H = \frac{\hbar^2\alpha^2}{2\mu}\,;\quad G_1 = \Lambda + \frac{\hbar^2\alpha^2\ell(\ell+1)}{2\mu}\,;\\
&G_2 = \frac{8\mu D_e a\lambda}{\hbar^2\alpha} - \frac{4\mu D_e a\lambda}{\hbar^2} + \frac{4\mu D_e a\gamma}{\hbar^2\alpha} - \ell(\ell+1).
\end{aligned}\right] \tag{23}$$

With the help of a Mathematica software, the partition function of the SSKP is obtained as

$$\begin{aligned}
Z(\beta, N_{\max}) = \frac{1}{2\sqrt{-H\beta}} e^{-\frac{\beta}{2}\left(\begin{smallmatrix}2G_1 + G_2 H\\ +H\sqrt{1+G_2^2}\end{smallmatrix}\right)} \sqrt{\pi}\left(\begin{aligned}&Erf\left[\frac{\sqrt{-G_2^2 H\beta} - \sqrt{-H\beta}\,\delta^2}{2\delta}\right]\\ &+Erf\left[\frac{-\sqrt{-G_2^2 H\beta} + \sqrt{-H\beta}\,(\delta + N_{\max})^2}{2(\delta + N_{\max})}\right]\end{aligned}\right)\\
+\frac{1}{2\sqrt{-H\beta}} e^{-\frac{\beta}{2}\left(\begin{smallmatrix}2G_1 + G_2 H\\ +H\sqrt{1+G_2^2}\end{smallmatrix}\right)} \sqrt{\pi}\, e^{H\beta\sqrt{1+G_2^2}}\left(\begin{aligned}&-Erf\left[\frac{\sqrt{-G_2^2 H\beta} + \sqrt{-H\beta}\,\delta^2}{2\delta}\right]\\ &+Erf\left[\frac{\sqrt{-G_2^2 H\beta} + \sqrt{-H\beta}\,(\delta + N_{\max})^2}{2(\delta + N_{\max})}\right]\end{aligned}\right),
\end{aligned} \tag{24}$$

where $N_{\max} = \sqrt{-G_2} - \delta$ and Erf denote the error function [43]. Other thermodynamic properties including free energy, internal energy, entropy, and specific heat capacity can be obtained using the following expressions [44]:

$$\left.\begin{aligned}
&F(\beta, N_{\max}) = -\frac{1}{\beta}\ln Z(\beta, N_{\max}), U(\beta, N_{\max}) = -\frac{d\ln Z(\beta, N_{\max})}{d\beta},\\
&S(\beta, N_{\max}) = \ln Z(\beta, N_{\max}) - \beta\frac{d\ln Z(\beta, N_{\max})}{d\beta}, C_v(\beta, N_{\max}) = \beta^2\frac{d^2\ln Z(\beta, N_{\max})}{d\beta^2}\ .
\end{aligned}\right] \tag{25}$$

Results and discussions

In this study, four diatomic molecule systems were considered. The spectroscopic parameters for the selected molecules are presented in Table 1, as obtained from Ref. [45]. The analytical expression for the energy eigenvalues of the SSKP model is given in Eq. (18). Numerical energy results of the SSKP for the selected diatomic molecules have been computed using the Maple software protocols. These results are presented in Tables 2–5, for various combinations of the

TABLE 1 Spectroscopic parameters for the selected diatomic molecule systems [45].

Molecules	$D_e\ (eV)$	$r_e\ (\mathring{A})$	$\mu\ (a.m.u.)$	$\alpha\ (\mathring{A}^{-1})$
H_2	4.7446	0.7416	0.50391	1.440558
LiH	2.515287	1.5956	0.8801221	1.7998368
HCl	4.61907	1.2746	0.9801045	2.3807
CO	11.2256	1.1283	0.6806719	2.59441

shifted parameters. It is worth mentioning here that the following conversions have been adopted throughout our computations: $\hbar c = 1973.296\ \text{eV}\mathring{A}$ and $1\ amu = 931.494028\ \text{MeV}c^{-2}$. It is observed that at a specific value of the vibrational quantum number n, the energy eigenvalues of the SSKP increase with an increase in the rotational quantum number l for the selected diatomic molecule system. This increase in the energy eigenvalues tends to remain constant with further increase in l, as will be demonstrated graphically in this article. Conversely, the energy eigenvalues of the selected systems are seen to decrease with an increase in n. These energy–quantum number relationships are observed in all the tables, as regards the shifted parameter pairs considered. The energy values of the SSKP for the selected diatomic molecules are very close to zero in the absence of the shifted parameters (when $\lambda = \gamma = 0$). As either of the shifted parameters is introduced, the energy eigenvalues begin to increase negatively. In the presence of both shifted parameters, the energy eigenvalues are seen to decrease tangibly for all the selected diatomic molecule systems.

The variations of the energy eigenvalues of the SSKP with different potential parameters and quantum numbers were considered. Throughout our graphical analysis, the following quantum numbers have been adopted: $n = 2;\ l = 1$. In Figure 1, a direct decrease in energy eigenvalues is observed as the dissociation increases for the selected systems. A monotonous decrease in the energy eigenvalues of the SSKP is observed as the equilibrium bond length increases as shown in Figure 2. This same trend is also seen in Figure 3 as the energy eigenvalues of the SSKP vary with the screening parameter. In Figure 4, the energy eigenvalues of the SSKP increase with the increase in the reduced mass for the selected diatomic molecule system. Thereafter, we observe constant values for the energy as the reduced mass further increases. A monotonous decrease is observed in the energy eigenvalues as the vibrational quantum number increases in Figure 5. In addition, the energy eigenvalues of the SSKP begin to increase with the increase in the rotational quantum number (Figure 6). As the rotational quantum number increases further, we observed that the energy eigenvalues of the SSKP remain constant at unique values for the selected systems. It is worth noting that the aforementioned graphical analyses were done in the presence of both the shifted parameters $(\lambda = \gamma = 1)$.

Furthermore, the variation of different thermodynamic properties of the SSKP with both temperature and maximum quantum number has been evaluated. These were done with the help of the partition function expression obtained in Eq. 24 and other thermodynamic expressions given in Eq. 25.

In Figure 7, we observe a sharp decrease in the partition function of the SSKP at zero temperature for the H_2 diatomic molecule, but a sharp increase in the partition functions of the SSKP are observed for LiH and HCl diatomic molecules. As the temperature increases, the partition functions of these diatomic molecules remain zero. The partition function of the

TABLE 2 Energy eigenvalues $(-E_{nl}\ (eV))$ of the shifted screened Kratzer potential for H_2.

n	l	$\lambda = 1,\ \gamma = 1$	$\lambda = 1,\ \gamma = 0.5$	$\lambda = 0,\ \gamma = 1$	$\lambda = 0,\ \gamma = 0.5$	$\lambda = 0,\ \gamma = 0$
0	0	12.88868820	12.76416270	0.8992448746	0.4240223638	0.002151891095
	1	12.86827450	12.74617456	0.8654425337	0.3909585419	0.002151891100
	2	12.82757504	12.71033331	0.7984648176	0.3260367213	0.002151891080
	3	12.76684367	12.65690644	0.6995367316	0.2315599492	0.002151891100
1	0	12.82620770	12.75708960	0.6750029392	0.2776908018	0.008607564380
	1	12.80673214	12.73997903	0.6440461866	0.2484289305	0.01171585151
	2	12.76790041	12.70588327	0.5826869799	0.1909215429	0.01344931932
	3	12.70994948	12.65505067	0.4920090164	0.1071130964	0.01454678380
2	0	12.78441944	12.76712128	0.4909923166	0.1684659411	0.01936701986
	1	12.76581972	12.75082670	0.4625452209	0.1424043945	0.02636066591
	2	12.72873192	12.71835413	0.4061433788	0.0911455039	0.03107330739
	3	12.67337754	12.66993457	0.3227499235	0.0163451509	0.03443025750
3	0	12.76194202	12.79308527	0.3422748993	0.09031887720	0.03443025752
	1	12.74416180	12.77755139	0.3160543843	0.06698185026	0.04553401557
	2	12.70870585	12.74659223	0.2640525401	0.02104828359	0.05379727740
	3	12.65578155	12.70042300	0.1871289623	−0.04606103475	0.06012120220

TABLE 3 Energy eigenvalues $(-E_{nl}\ (eV))$ of the shifted screened Kratzer potential for *LiH*.

n	l	$\lambda = 1,\ \gamma = 1$	$\lambda = 1,\ \gamma = 0.5$	$\lambda = 0,\ \gamma = 1$	$\lambda = 0,\ \gamma = 0.5$	$\lambda = 0,\ \gamma = 0$
0	0	20.66232586	21.78971193	0.5308115944	0.2767741104	0.001923247146
	1	20.65827201	21.78663642	0.5199423639	0.2659913923	0.001923247160
	2	20.65017029	21.78049083	0.4982516798	0.2445201457	0.001923247160
	3	20.63803260	21.77128598	0.4658345730	0.2125466994	0.001923247220
1	0	21.01184393	22.10611604	0.6429174044	0.3586710210	0.007692988585
	1	21.00783785	22.10307007	0.6324165656	0.3483980377	0.01047101224
	2	20.99983153	22.09698342	0.6114601496	0.3279393678	0.01202029467
	3	20.98783657	22.08786667	0.5801381824	0.2974677432	0.01300115075
2	0	21.36521806	22.42648181	0.7638658892	0.4491866256	0.01730922432
	1	21.36125959	22.42346597	0.7537156257	0.4393895494	0.02355977755
	2	21.35334835	22.41743948	0.7334580148	0.4198764468	0.02777168880
	3	21.34149564	22.40841261	0.7031784186	0.3908077276	0.03077195445
3	0	21.72244784	22.75080389	0.8932997882	0.5478522930	0.03077195434
	1	21.71853683	22.74781876	0.8834836786	0.5385009259	0.04069590962
	2	21.71072035	22.74185354	0.8638921870	0.5198735695	0.04808117867
	3	21.69900944	22.73291826	0.8346063258	0.4921194260	0.05373317035

TABLE 4 Energy eigenvalues $(-E_{nl}\ (eV))$ of the shifted screened Kratzer potential for *HCl*.

n	l	$\lambda = 1,\ \gamma = 1$	$\lambda = 1,\ \gamma = 0.5$	$\lambda = 0,\ \gamma = 1$	$\lambda = 0,\ \gamma = 0.5$	$\lambda = 0,\ \gamma = 0$
0	0	53.03004677	55.21501868	1.339228248	0.6916973618	0.003021681800
	1	53.02412415	55.21057543	1.322852179	0.6754326794	0.003021681800
	2	53.01228562	55.20169491	1.290155296	0.6430124931	0.003021681800
	3	52.99454449	55.18838917	1.241247644	0.5946533158	0.003021681800
1	0	53.65699039	55.77699589	1.555655962	0.8486391966	0.01208672720
	1	53.65112485	55.77258552	1.539760989	0.8330422482	0.01645137868
	2	53.63940031	55.76377071	1.508023752	0.8019505234	0.01888551125
	3	53.62182986	55.75056320	1.460549228	0.7555666792	0.02042656900
2	0	54.28997836	56.34535428	1.785256510	1.018471857	0.02719513620
	1	54.28416993	56.34097778	1.769822458	1.003504085	0.03701560205
	2	54.27255952	56.33223053	1.739004669	0.9736642888	0.04363308520
	3	54.25515986	56.31912407	1.692903350	0.9291424076	0.04834690880
3	0	54.92901063	56.92008005	2.027579578	1.200599368	0.04834690880
	1	54.92325938	56.91573831	2.012587664	1.186225879	0.06393878689
	2	54.91176316	56.90706045	1.982651897	1.157568739	0.07554204500
	3	54.89453447	56.89405776	1.937868003	1.114806194	0.08442208950

CO diatomic molecule increases monotonously from a certain temperature and it approaches zero as the temperature increases. The free energy of the SSKP for the selected diatomic molecule systems is seen to decrease with an increase in temperature, as shown in Figure 8.

In Figure 9, there exists a monotonous decrease in the internal energy of the SSKP for the selected diatomic molecule systems toward zero as the temperature increases.

The plot of entropy of the SSKP with temperature is shown in Figure 10 for the diatomic molecule systems considered. Here, the entropies of the diatomic molecules increase to unique values, corresponding to a selected diatomic molecule system at a particular temperature. This temperature value corresponding to the peak values of entropy is called the critical temperature. As the temperature increases further, the entropy values begin to decrease gradually. With further increase in the temperature, the entropy of the selected systems remains constant.

The specific heat capacities of the SSKP for the selected diatomic molecules are seen to increase monotonously as the temperature increases first (Figure 11). With further increase in

TABLE 5 Energy eigenvalues $(-E_{nl}\ (eV))$ of the shifted screened Kratzer potential for *CO*.

n	l	$\lambda = 1,\ \gamma = 1$	$\lambda = 1,\ \gamma = 0.5$	$\lambda = 0,\ \gamma = 1$	$\lambda = 0,\ \gamma = 0.5$	$\lambda = 0,\ \gamma = 0$
0	0	127.2547770	132.4419189	2.472618737	1.248758647	0.0005126516235
	1	127.2537190	132.4411200	2.469726022	1.245871077	0.0005126516240
	2	127.2516029	132.4395221	2.463941362	1.240097394	0.0005126516300
	3	127.2484290	132.4371256	2.455266197	1.231440555	0.0005126516300
1	0	127.6403250	132.7893135	2.593471190	1.334926081	0.002050606494
	1	127.6392699	132.7885163	2.590602477	1.332072278	0.002791103281
	2	127.6371595	132.7869220	2.590602477	1.326366104	0.003204072650
	3	127.6339945	132.7845305	2.576262607	1.317810460	0.003465524980
2	0	128.0268992	133.1377746	2.716745726	1.423499826	0.004613864612
	1	128.0258469	133.1369792	2.713900721	1.420679214	0.006279982392
	2	128.0237424	133.1353884	2.708211461	1.415039392	0.007402689450
	3	128.0205861	133.1330022	2.699679347	1.406583212	0.008202425980
3	0	128.4144994	133.4873018	2.842417020	1.514444733	0.008202425976
	1	128.4134500	133.4865082	2.839595433	1.511656748	0.01084770835
	2	128.4113514	133.4849208	2.833953009	1.506082157	0.01281629059
	3	128.4082038	133.4825398	2.825491122	1.497723759	0.01432285864

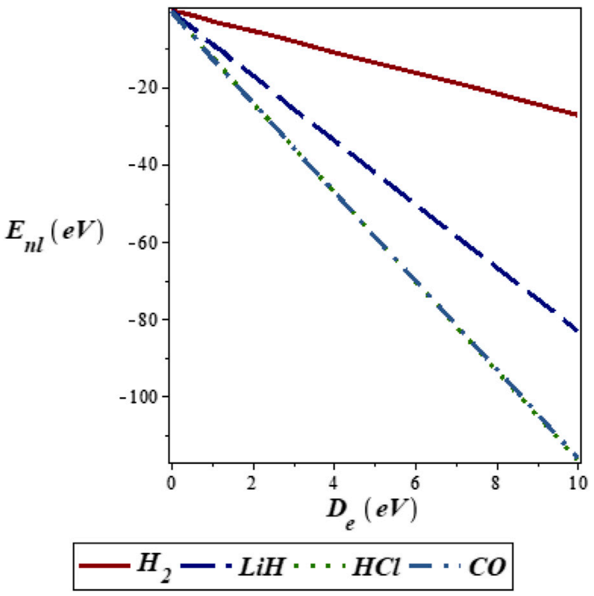

FIGURE 1
Variation of energy eigenvalues of the SSKP with dissociation energy for different diatomic molecule systems with n = 2 and l = 1.

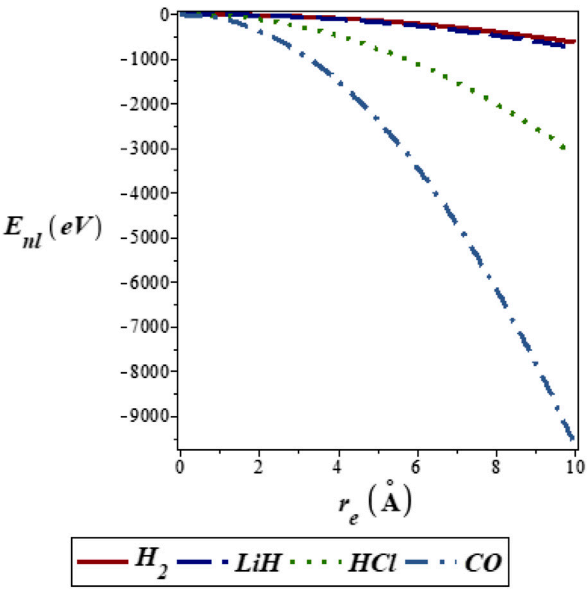

FIGURE 2
Variation of energy eigenvalues of the SSKP with equilibrium bond length for different diatomic molecule systems with n = 2 and l = 1.

the temperature beyond a certain value, the specific heat capacity values for the molecule systems considered remain constant around zero.

Figure 12 shows the variation of the partition function of the SSKP with maximum vibration quantum number for the selected molecule systems. The partition function here increases with an increase in the maximum vibration quantum number. In Figure 13, the free energy of the SSKP for the selected molecule systems decreases monotonously with the increase in the maximum vibration quantum number. The variation of the internal energy of the SSKP for the different diatomic molecule systems is shown in Figure 14. In this plot, the internal energies for the selected molecule systems first increase slowly at a

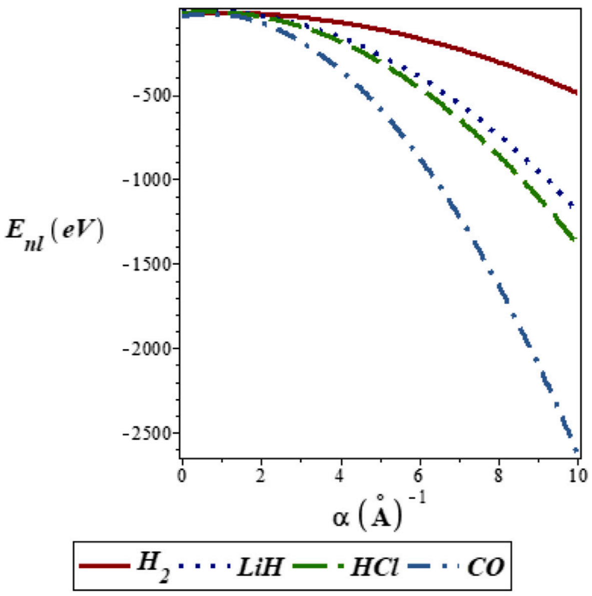

FIGURE 3
Variation of energy eigenvalues of the SSKP with screening parameters for different diatomic molecule systems with $n = 2$ and $l = 1$.

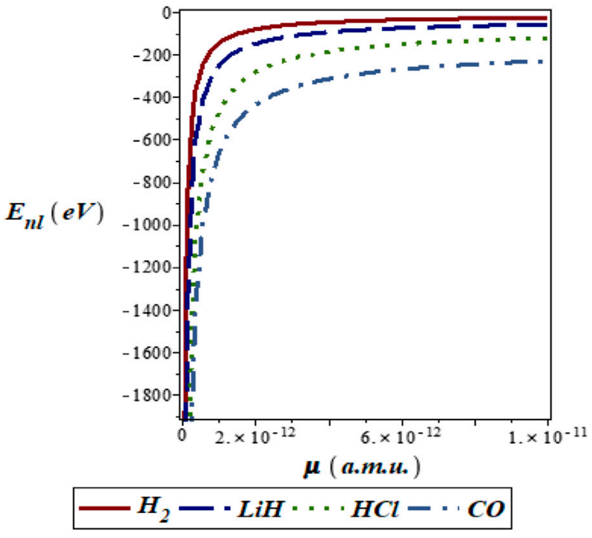

FIGURE 4
Variation of energy eigenvalues of the SSKP with reduced mass for different diatomic molecule systems with $n = 2$ and $l = 1$.

particular value of the maximum vibration quantum number. With the further enhancement of the maximum vibration quantum number, the internal energies of these diatomic systems begin to decrease monotonously at different paces. Figure 15 shows a monotonous increase in the entropy of the SSKP for the different diatomic molecule systems as the maximum vibration quantum number increases.

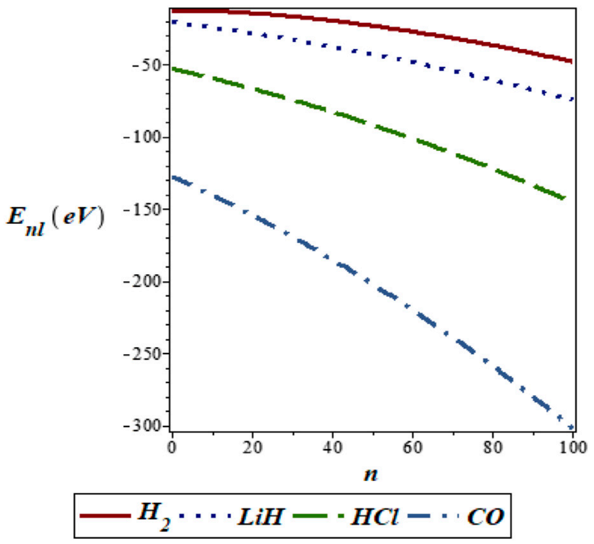

FIGURE 5
Variation of energy eigenvalues of the SSKP with vibrational quantum number for different diatomic molecule systems with $l = 1$.

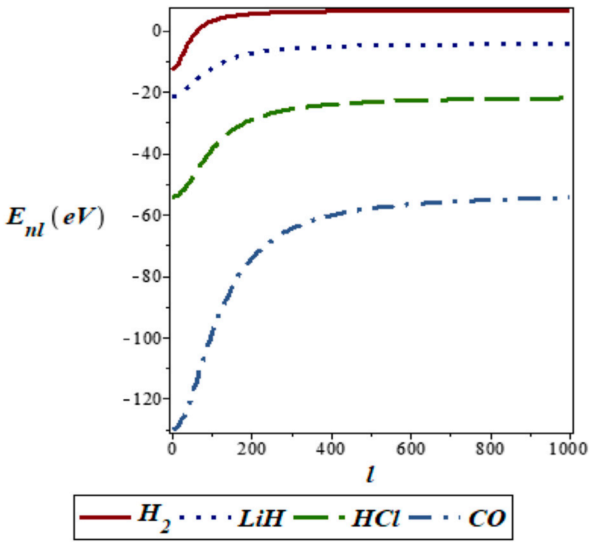

FIGURE 6
Variation of energy eigenvalues of the SSKP with rotational quantum number for different diatomic molecule systems with $n = 2$.

In Figure 16, the specific heat capacity of the SSKP is also seen to increase with the increase in the maximum vibration quantum number for the diatomic molecule systems considered. Our results obtained are seen to agree perfectly with previous

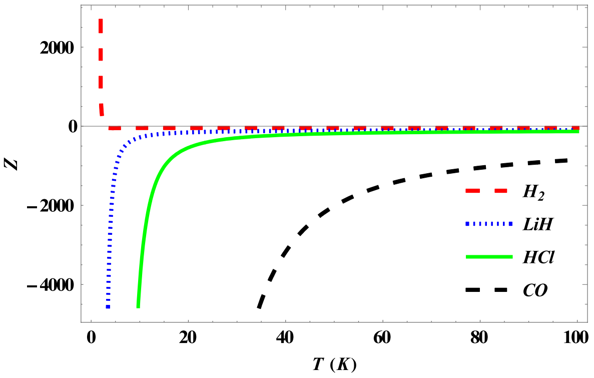

FIGURE 7
Variation of the partition function of the SSKP with temperature for different diatomic molecule systems with $n = 2$ and $l = 1$.

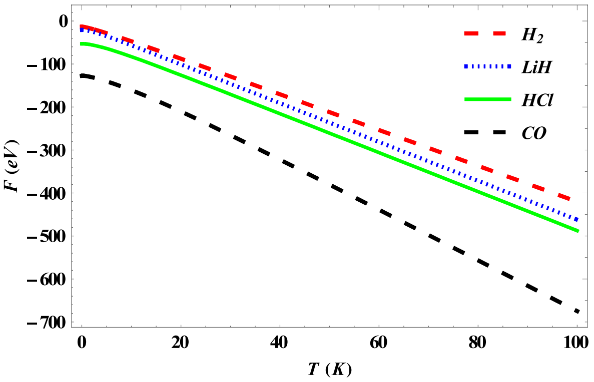

FIGURE 8
Variation of free energy of the SSKP with temperature for different diatomic molecule systems with $n = 2$ and $l = 1$.

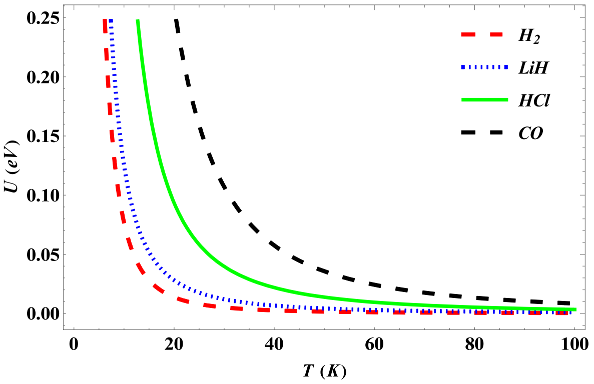

FIGURE 9
Variation of internal energy of the SSKP with temperature for different diatomic molecule systems with $n = 2$ and $l = 1$.

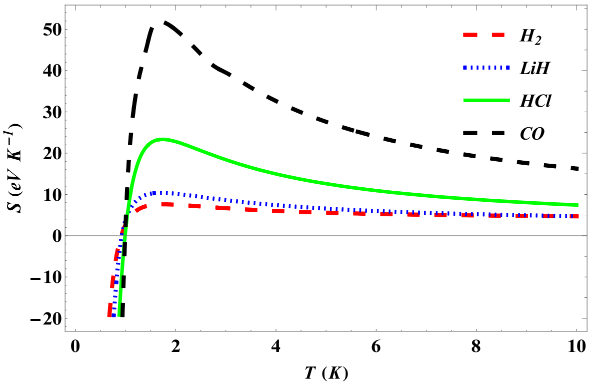

FIGURE 10
Variation of entropy of the SSKP with temperature for different diatomic molecule systems with $n = 2$ and $l = 1$.

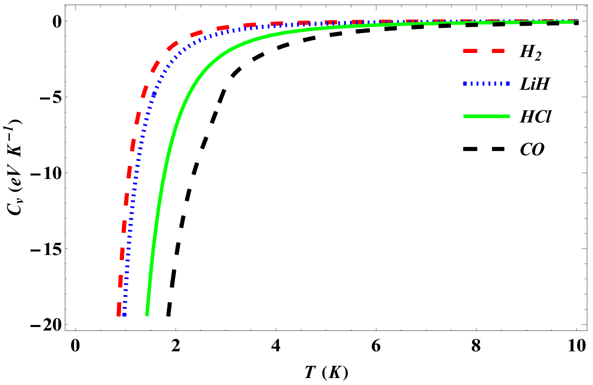

FIGURE 11
Variation of the specific heat capacity of the SSKP with temperature for different diatomic molecule systems with $n = 2$ and $l = 1$.

studies [34], as regards the selected diatomic molecule systems [44].

Concluding remarks

In this work, the extended Nikiforov–Uvarov method (ENU) was employed to solve the radial Schrodinger equation for the shifted screened Kratzer potential (SSKP) model and its analytical expression of energy eigenvalues was obtained. With the help of the energy eigenvalues, the expression for the partition function and other thermodynamic properties' expressions were obtained using the exact method. In this

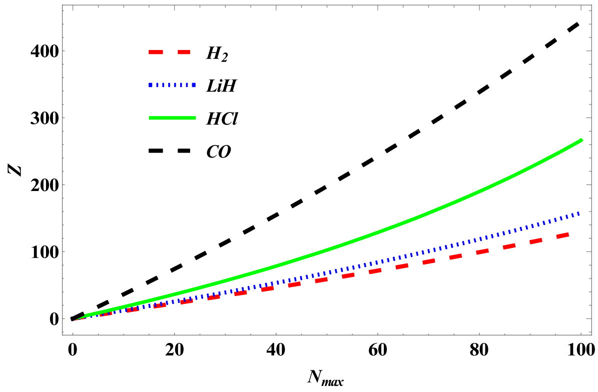

FIGURE 12
Variation of the partition function of SSKP with maximum vibration quantum number for different diatomic molecule systems with n = 2 and l = 1.

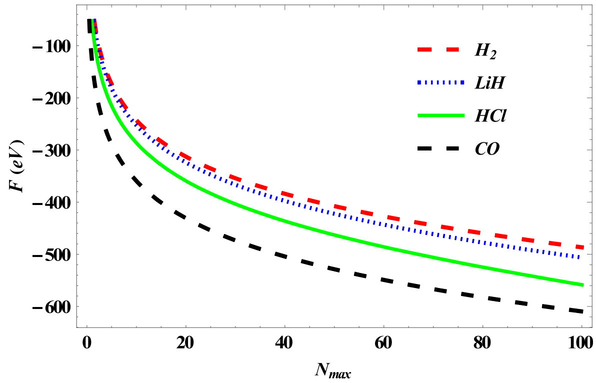

FIGURE 13
Variation of free energy of the SSKP with maximum vibration quantum number for different diatomic molecule systems with n = 2 and l = 1.

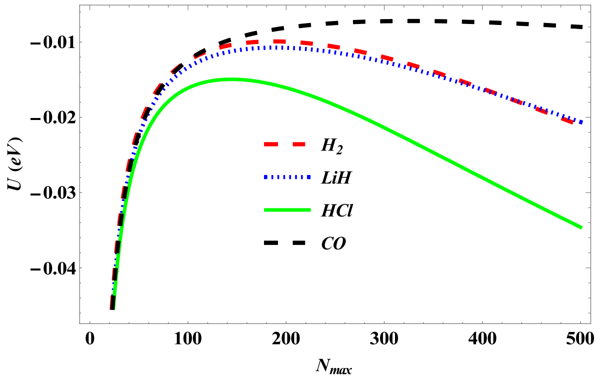

FIGURE 14
Variation of internal energy of the SSKP with maximum vibration quantum number for different diatomic molecule systems with n = 2 and l = 1.

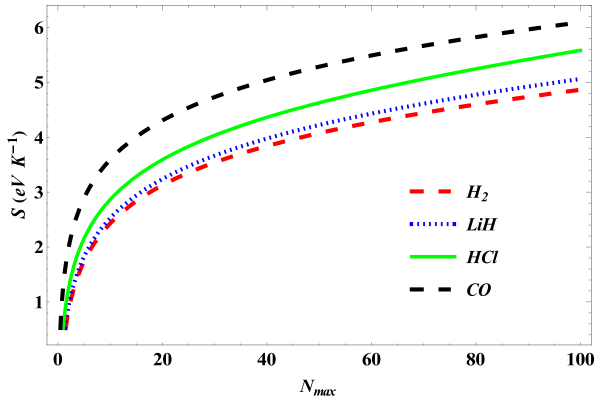

FIGURE 15
Variation of entropy of the SSKP with maximum vibration quantum number for different diatomic molecule systems with n = 2 and l = 1.

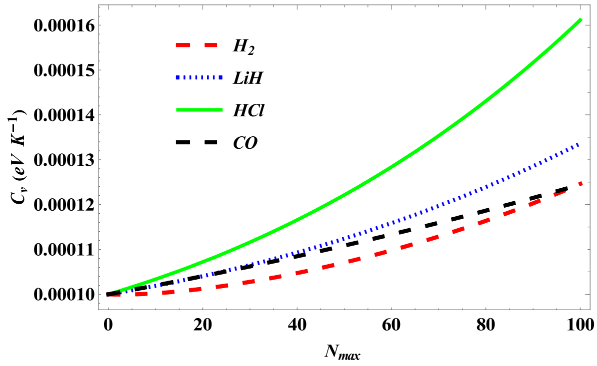

FIGURE 16
Variation of specific heat capacity of the SSKP with maximum vibration quantum number for different diatomic molecule systems with n = 2 and l = 1.

study, four different diatomic molecule systems were employed. These were hydrogen dimer, lithium hydride molecule, hydrogen chloride molecule, and carbon monoxide molecule. With the help of spectroscopic parameters of the selected diatomic molecule systems extracted from available literatures, numerical results of energies of the SSKP were obtained at different quantum states and shifted parameters. The shifted parameters were seen to have a great effect on the energy eigenvalues obtained. In addition, variations of the energy eigenvalues of the SSKP with different potential parameters and quantum numbers were analyzed graphically.

Furthermore, the variations of the partition function and other thermodynamic properties of the SSKP with respect to temperature and maximum vibration quantum number for the diatomic molecule systems considered were studied graphically.

The major result obtained lies in the existence of the critical temperature for each of the diatomic molecule system considered. From our results, the SSKP model can be employed to predict the thermochemical properties of different diatomic molecule systems. It is our future intention to study the higher dimensional energies of these diatomic molecule systems in the relativistic regime.

Data availability statement

The raw data supporting the conclusion of this article will be made available by the authors, without undue reservation.

Author contributions

All the authors contributed to the manuscript as follows: 1) NI conceptualized the idea. 2) UO wrote the first draft and computed the thermodynamic functions. 3) NS carried out the literature analysis. 4) MR discussed all the results. 5) GR conducted the proof reading and corrected all the necessary corrections.

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Publisher's note

References

1. Dong SH. *Factorization method in quantum mechanics*. Armsterdam: Springer (2007).

2. Liu JY, Zhang GD, Jia CS. Calculation of the interaction potential energy curve and vibrational levels for the state of molecule. *Phys Lett A* (2013) 377:1444–7. doi:10.1016/j.physleta.2013.04.019

3. Nikiforov AF, Uvarov VB, *Special functions of mathematical physics* (Germany: Birkhauser Verlag Basel), A Jaffe, 317 (1988).

4. Ciftci H, Hall RL, Saad N. Construction of exact solutions to eigenvalue problems by the asymptotic iteration method. *J Phys A: Math Gen* (2005) 38: 1147–55. doi:10.1088/0305-4470/38/5/015

5. Ikot AN, Okorie US, Amadi PO, Edet CO, Rampho GJ, Sever R. *Few body syst*, 62. Berlin, Germany: Springer (2020). p. 9.

6. Karayer H, Demirhan D, Buyukkilic F. Extension of Nikiforov-Uvarov method for the solution of Heun equation. *J Math Phys* (2015) 56:063504. doi:10.1063/1.4922601

7. Witten E. Dynamical breaking of supersymmetry. *Nucl Phys B* (1981) 188: 513–54. doi:10.1016/0550-3213(81)90006-7

8. Ma ZQ, Xu BW. Quantum correction in exact quantization rules. *Europhys Lett* (2005) 69:685–91. doi:10.1209/epl/i2004-10418-8

9. Castro E, Paz JL, Martin P. Analytical approximations to the eigenvalues of the Morse potential with centrifugal terms. *J Mol Struct THEOCHEM* (2006) 769:15–8. doi:10.1016/j.theochem.2005.11.034

10. Jia CS, Diao YF, Liu XJ, Wang PQ, Liu JY, Zhang GD. Equivalence of the Wei potential model and Tietz potential model for diatomic molecules. *J Chem Phys* (2012) 137:014101. doi:10.1063/1.4731340

11. Jia CS, Yi LZ, Long SW. Relationship of the deformed hyperbolic Kratzer-like and Tietz potential energy models for diatomic molecules. *Can J Phys* (2014) 92: 1258–61. doi:10.1139/cjp-2013-0684

12. Gao J, Zhang MC. Analytical solutions to the D-dimensional Schrödinger equation with the Eckart potential. *Chin Phys Lett* (2016) 33:010303. doi:10.1088/0256-307X/33/1/010303

13. Liu L, Rana J, Liao S. Analytical solutions for the hydrogen atom in plasmas with electric, magnetic, and Aharonov-Bohm flux fields. *Phys Rev E* (2021) 103: 023206. doi:10.1103/physreve.103.023206

14. Solaimani M, Dong SH. Quantum information entropies of multiple quantum well systems in fractional Schrödinger equations. *Int J Quan Chem* (2020) 120: e26113. doi:10.1002/qua.26113

15. Shi YJ, Sun GH, Tahir F, Ahmadov AI, He B, Dong SH. Quantum information measures of infinite spherical well. *Mod Phys Lett A* (2018) 33:1850088. doi:10.1142/s0217732318500888

16. Isonguyo CN, Oyewumi KJ, Oyun OS. Quantum information-theoretic measures for the static screened Coulomb potential. *Int J Quan Chem* (2018) 118:025620. doi:10.1002/qua.25620

17. Onate CA, Ikot AN, Onyeaju MC, Ebomwonyi O, Idiodi JOA. Effect of dissociation energy on Shannon and Rényi entropies. *Karbala Int J Mod Sci* (2018) 4:134–42. doi:10.1016/j.kijoms.2017.12.004

18. Amadi PO, Ikot A. N, Ngiangia AT, Okorie US, Rampho GJ, Abdullah HY. Shannon entropy and Fisher information for screened Kratzer potential. *Int J Quan Chem* (2020) 120:e26246. doi:10.1002/qua.26246

19. Chabi K, Boumali A. Thermal properties of three dimensional Morse potential for some diatomic molecules via Euler-Maclaurin approximation. *Rev Mex Fis* (2020) 66:110–20. doi:10.31349/revmexfis.66.110

20. Ikot AN, Azogor W, Okorie US, Bazuaye FE, Onyeaju MC, Onate CA, et al. Exact and Poisson summation thermodynamic properties for diatomic molecules with shifted Tietz potential. *Indian J Phys* (2019) 93:1171–9. doi:10.1007/s12648-019-01375-0

21. Edet CO, Okorie US, Osobonye G, Ikot AN, Rampho GJ, Sever R. Thermal properties of Deng–Fan–Eckart potential model using Poisson summation approach. *J Math Chem* (2020) 58:989–1013. doi:10.1007/s10910-020-01107-4

22. Okorie US, Ikot AN, Onyeaju MC, Chukwuocha EO. A study of thermodynamic properties of quadratic exponential-type potential in D-dimensions. *Rev Mex Fis* (2018) 64:608–614.

23. Okorie US, Ikot AN, Chukwuocha EO, Rampho GJ. Thermodynamic properties of improved deformed exponential-type potential (IDEP) for some diatomic molecules. *Results Phys* (2020) 17:103078. doi:10.1016/j.rinp.2020.103078

24. Jia CS, Zhang LH, Wang CW. Thermodynamic properties for the lithium dimer. *Chem Phys Lett* (2017) 667:211–5. doi:10.1016/j.cplett.2016.11.059

25. Song XQ, Wang CW, Jia CS. Thermodynamic properties for the sodium dimer. *Chem Phys Lett* (2017) 673:50–5. doi:10.1016/j.cplett.2017.02.010

26. Jia CS, Wang CW, Zhang LH, Peng XL, Zeng R, You XT. Partition function of improved Tietz oscillators. *Chem Phys Lett* (2017) 676:150–3. doi:10.1016/j.cplett.2017.03.068

27. Al-Jamel A. Saturation in heavy quarkonia spectra with energy-dependent confining potential in *N*-dimensional space. *Mod Phys Lett A* (2018) 32:1850185. doi:10.1142/s0217732318501857

28. Chaturvedi R, Rai AK. Charmonium spectroscopy motivated by general features of pNRQCD. *Int J Theor Phys (Dordr)* (2020) 59:3508–32. doi:10.1007/s10773-020-04613-y

29. Kher V, Rai AK. Spectroscopy and decay properties of charmonium. *Chin Phys C* (2018) 42:083101. doi:10.1088/1674-1137/42/8/083101

30. Ibekwe EE, Okorie US, Emah JB, Inyang EP, Ekong SA. Mass spectrum of heavy quarkonium for screened Kratzer potential (SKP) using series expansion method. *Eur Phys J Plus* (2021) 136:87. doi:10.1140/epjp/s13360-021-01090-y

31. Qiang WC, Hong-Hong C. *Ab initio* calculations of electronic structure of anatase TiO_2. *Chin Phys* (2004) 13:2121–5. doi:10.1088/1009-1963/13/12/025

32. Rampho GJ, Ikot AN, Edet CO, Okorie US. Energy spectra and thermal properties of diatomic molecules in the presence of magnetic and AB fields with improved Kratzer potential. *Mol Phys* (2021) 119:e1821922. doi:10.1080/00268976.2020.1821922

33. Ikot AN, Okorie US, Sever R, Rampho GJ. Eigensolution, expectation values and thermodynamic properties of the screened Kratzer potential. *Eur Phys J Plus* (2019) 134:386. doi:10.1140/epjp/i2019-12783-x

34. Ikot AN, Okorie US, Rampho GJ, Amadi PO, Edet CO, Akpan IO, et al. Klein–gordon equation and nonrelativistic thermodynamic properties with improved screened kratzer potential. *J Low Temp Phys* (2021) 202:269–89. doi:10.1007/s10909-020-02544-w

35. Onate CA, Onyeaju MC, Ikot AN, Ebomwonyi O. Eigen solutions and entropic system for Hellmann potential in the presence of the Schrödinger equation. *Eur Phys J Plus* (2017) 132:462. doi:10.1140/epjp/i2017-11729-8

36. Zhang LH, Li XP, Jia CS. Approximate solutions of the Schrödinger equation with the generalized Morse potential model including the centrifugal term. *Int J Quan Chem* (2011) 111:1870–8. doi:10.1002/qua.22477

37. Greene RL, Aldrich C. Variational wave functions for a screened Coulomb potential. *Phys Rev A (Coll Park)* (1976) 143:2363–6. doi:10.1103/physreva.14.2363

38. Karayer H, Demirhan D, Buyukkilic F. Solution of Schrödinger equation for two different potentials using extended Nikiforov-Uvarov method and polynomial solutions of biconfluent Heun equation. *J Math Phys* (2018) 59:053501. doi:10.1063/1.5022008

39. Karayer H, Demirhan D, Buyukkilic F. Some special solutions of biconfluent and triconfluent heun equations in elementary functions by extended nikiforov–uvarov method. *Rep Math Phys* (2015) 76:271–81. doi:10.1016/s0034-4877(15)00039-7

40. Servatkhah M, Khordad R, Ghanbari A. Accurate prediction of thermodynamic functions of H2 and LiH using theoretical calculations. *Int J Thermophys* (2020) 41:37. doi:10.1007/s10765-020-2615-0

41. Horchani R, Jelassi H. Effect of quantum corrections on thermodynamic properties for dimers. *Chem Phys* (2020) 532:110692. doi:10.1016/j.chemphys.2020.110692

42. Khordad R, Ghanbari A. Theoretical prediction of thermodynamic functions of TiC: Morse ring-shaped potential. *J Low Temp Phys* (2020) 199:1198–210. doi:10.1007/s10909-020-02368-8

43. Ikot AN, Chukwuocha EO, Onyeaju MC, Onate CA, Ita BI, Udoh ME. Thermodynamics properties of diatomic molecules with general molecular potential. *Pramana - J Phys* (2018) 90:22. doi:10.1007/s12043-017-1510-0

44. Osobonye GT, Adekanmbi M, Ikot AN, Okorie US, Rampho GJ, Pramana J. Thermal properties of anharmonic Eckart potential model using Euler–MacLaurin formula. *Pramana - J Phys* (2021) 95:98. doi:10.1007/s12043-021-02122-z

45. Nasser I, Abdelmonem MS, Bahlouli H, Alhaidar A. The rotating morse potential model for diatomic molecules in the tridiagonal*J*-matrix representation: I. Bound states. *J Phys B: Mol Opt Phys* (2007) 40:4245–57. doi:10.1088/0953-4075/40/21/011

Appendix A: Extended Nikiforov–Uvarov method

The extended Nikiforov–Uvarov (ENU) method was proposed by [6, 38, 39] as an extended form of the Nikiforov–Uvarov (NU) method to transform Schrodinger-like equations into a second-order differential equation which has at most four singular points that can be solved analytically. The ENU method is defined as

$$\psi''(s) + \frac{\tilde{\tau}_e(s)}{\sigma_e(s)}\psi'(s) + \frac{\tilde{\sigma}_e(s)}{\sigma_e^{2}(s)}\psi(s) = 0, \tag{A1}$$

where $\tilde{\tau}_e(s)$, $\sigma_e(s)$, and $\tilde{\sigma}_e(s)$ are polynomials of at most second, third, and fourth degrees, respectively, and e stands for “extended.” Using the following transformation

$$\psi(s) = \phi_e(s)y_n(s), \tag{A2}$$

the basic equation given by Eq. A1 becomes a hypergeometric-type equation

$$\sigma_e(s)y''(s) + \tau_e(s)y'(s) + h(s)y(s) = 0. \tag{A3}$$

Eq. A3 has a particular polynomial solution of the form $y(s) = y_n(s)$ and the function $\phi_e(s)$ is given as a logarithmic derivative:

$$\frac{\phi_e'(s)}{\phi_e(s)} = \frac{\pi(s)}{\sigma(s),} \tag{A4}$$

with $\pi_e(s)$ being at most a second-degree polynomial. The second part of $\phi_e(s)$ being $y_n(s)$ in Eq. A2 is the hypergeometric function with its polynomial solution given by the Rodrigues relation,

$$y_n(s) = \frac{B_n}{\rho(s)}\frac{d^n}{ds^n}\left[\sigma^n(s)\rho(s)\right]. \tag{A5}$$

Here, B_n is the normalization constant and $\rho(s)$ is the weight function which must satisfy the condition

$$\frac{d}{ds}\left[\sigma(s)\rho(s)\right] = \tau(s)\rho(s), \tag{A6}$$

with

$$\tau_e(s) = \tilde{\tau}_e(s) + 2\pi_e(s). \tag{A7}$$

The polynomials $\tau_e(s)$, $\pi_e(s)$, and $h(s)$ arising in the procedure of reducing the basic equation of the method to Eq. A3 are defined as

$$\pi_e(s) = \frac{\sigma_e'(s) - \tilde{\tau}_e(s)}{2} \pm \sqrt{\left(\frac{\sigma_e'(s) - \tilde{\tau}_e(s)}{2}\right)^2 - \tilde{\sigma}_e(s) + G(s)\sigma_e(s)} \tag{A8}$$

and

$$h(s) = G(s) + \pi_e'(s), \tag{A9}$$

where

$$G(s) = Ps + Q. \tag{A10}$$

According to the condition that polynomial $\pi_e(s)$ is at most second degree, polynomial $G(s)$ must be chosen properly. After determination of polynomial $G(s)$, all newly defined polynomials can be achieved by using Eqs. A7, A8, A9. As such, the new eigenvalue equation can be given as

$$h(s) = h_n(s) = -\frac{n}{2}\tau_e'(s) - \frac{n(n-1)}{6}\sigma_e''(s) + C_n, \tag{A11}$$

where C_n is an integration constant.

But, if and only if $\pi_e(s)$ is a polynomial of degree at most one, the eigenvalue equation can be obtain from the conventional NU method of the form

$$h(s) = h_n(s) = -n\tau'(s) - \frac{n(n-1)}{2}\sigma''(s)\,(n = 0, 1, 2, \ldots). \tag{A12}$$