East European Journal of Physics. **3.** 32-38 (2022)
DOI:10.26565/2312-4334-2022-3-04 ISSN 2312-4334

THE STUDY OF ELECTRONIC STATES OF NI AND ScI MOLECULES WITH SCREENED KRATZER POTENTIAL[†]

Etido P. Inyang[a], Effiong O. Obisung[b]
[a]*Department of Physics, National Open University of Nigeria, Jabi, Abuja, Nigeria*
[b]*Department of Physics, University of Calabar, Calabar, Nigeria*
Corresponding author E-mail: etidophysics@gmail.com, einyang@noun.edu.ng
Received June 7, 2022; revised August 10, 2022; accepted August 14, 2022

In this study, the analytical solutions of the Schrödinger equation with the screened Kratzer potential model is solved using the well-known Nikiforov-Uvarov method. The energy spectrum and the normalized wave function with the Greene-Aldrich approximation to the centrifugal term are obtained. The energy spectrum is used to generate eigenvalues for $X^3\Sigma^-$ state of NI and $X^1\Sigma^+$ state of ScI molecules respectively. The calculated results agree excellently with the experimental data. This research finds application in chemistry, industry, molecular physics and studies on magnetocaloric effect for several molecules. Our findings also demonstrate that the approximation scheme is well suited for this potential.
Keywords: Schrödinger equation; Nikiforov-Uvarov method; screened Kratzer Potential; molecules
PACS: 31.15.-p

1. Introduction

The study of diatomic molecules and their positive ions with the Schrödinger equation (SE) over the years have attracted the interest of both experimental and theoretical scientist because of its importance in chemistry and physics [1,2]. This is because solutions of the SE contain information about the system [3]. The solutions of the SE with different diatomic potential functions have been investigated by many authors [4-6]. Also, to obtain the SE solutions different methods have been employed such as the Asymptotic iteration method (AIM) [7], Laplace transformation method [8], supersymmetric quantum mechanics (SUSYQM) [9], the Nikiforov-Uvarov (NU) method [10-15], the Nikiforov-Uvarov-Functional Analysis (NUFA) method [16], the series expansion method (SEM) [17,18], the analytical exact iterative method (AEIM) [19], the WKB approximation method [20,21] and so on.

Recently, many authors have devoted interest in investigating bound states energy of countless diatomic molecules (DMs) with a single potential function and a combined potential function [22-24]. For instance, Inyang et al. [25] used Eckart and Hellmann potential function to study some selected DMs. Also, Obogo et al. [26], investigated some selected DMs through the solution of SE with a combined potential using the NU method. Furthermore, Edet and Ikot [27] studied some DMs with Deng-Fan plus Eckart potentials. Apart from the above studies, the energies for cesium molecule, sodium dimer, nitrogen dimer, hydrogen molecules, and potassium with the improved Rosen-Morse, Morse, Tietz-Hua oscillator, and improved Poschl-Teller oscillator potentials have been calculated and the results for each molecule was seen to agree with the experimental data [28-31]. Motivated by the success of their reports, we seek to obtain the energies for $X^3\Sigma^-$ state of NI and $X^1\Sigma^+$ state of ScI molecules.

The screened Kratzer potential (SKP), proposed by Ikot et al. [32] is a molecular potential, which finds application in molecular physics and many authors have employed in literature [33-35].

The aim of this study is to obtain the solutions to the SE with the SKP and apply it to calculate the energy eigenvalues for $X^3\Sigma^-$ state of NI and $X^1\Sigma^+$ state of ScI. The SKP is of the form [32]:

$$V(p) = -\frac{A_2 e^{-\vartheta p}}{p} + \frac{A_3 e^{-\vartheta p}}{p^2}, \tag{1}$$

where ϑ is the screening parameter. The letter $A_2 \equiv 2D_e r_e$ and $A_3 \equiv D_e r_e^2$, here D_e is dissociation energy, p is radial distance and r_e is the equilibrium bond length.

2. The solutions of the SE with SKP

In this research, the NU method is adopted and the details of the NU can be found in Ref. [14].
The SE characterized by a given potential $V(p)$ reads [36]

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

[†] ***Cite as***: E.P. Inyang, and E.O. Obisung, East Eur. J. Phys. **3**, 32 (2022), https://doi.org/10.26565/2312-4334-2022-3-04

where $\Psi_{nl}(p)$ is the Eigen functions, E_{nl} is the energy, μ is the reduced mass, $\hbar$ is the reduced Planck's constant and p is radial distance.

Substituting Eq. (1) into Eq. (2) gives Eq. (3),

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

Equation (3), is solved with the approximation scheme (AS) proposed by Greene-Aldrich [37] to deal with the centrifugal barrier. This AS is a good approximation to the centrifugal barrier which is valid for $\vartheta \ll 1,$ and its reads [38]

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

Plugging Eq. (4) into Eq. (3), Eq. (5) is:

$$\frac{d^2\psi_{nl}(p)}{dp^2}+\left[\frac{2\mu E_{nl}}{\hbar^2}+\frac{2\mu A_2\vartheta e^{-\vartheta p}}{\hbar^2\left(1-e^{-\vartheta p}\right)}-\frac{2\mu A_3\vartheta^2 e^{-\vartheta p}}{\hbar^2\left(1-e^{-\vartheta p}\right)^2}-\frac{\vartheta^2 l(l+1)}{\left(1-e^{-\vartheta p}\right)^2}\right]\psi_{nl}(p)=0\,. \tag{5}$$

We set

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

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

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

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

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

where

$$\left.-\varepsilon=\frac{2\mu E_{nl}}{\vartheta^2\hbar^2},\quad \eta_0=\frac{2\mu A_2}{\vartheta\hbar^2},\quad \eta_1=\frac{2\mu A_3}{\hbar^2},\quad \gamma=l(l+1)\right\}. \tag{9}$$

Linking Eq. (8) and Eq. (1) of Ref. [14], we have:

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

Inserting Eq. (10) into Eq. (11) of Ref. [14], gives:

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

where

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

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

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

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

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

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

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

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

where $\tau'(y)$ is the first derivative of $\tau(y)$. Referring to Eq. (10) and Eq. (13) of Ref. [14], we have λ_n and λ as follows:

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

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

When linking Eqs. (17) and (18) and substituting Eq. (9), the energy equation for the SKP is gotten as:

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

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

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

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

Putting Eqs. (10) and (21), into Eq. (2) of Ref. [14], the Rodrigues relation is written as

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

where B_n is the Jacobi polynomial. Hence,

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

where N_{nl} is the normalization constant, with the condition, we have:

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

where

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

Linking Eq. (26) with Eq. (37) of Ref. [39], we obtain:

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

Hereafter, the normalization constant is

$$\mathrm{N}_{nl}=\left[\frac{n!2\sqrt{B_3}\ \vartheta\,\Gamma\left(2\sqrt{B_3}+2\sqrt{B_3+B_2+B_1}+n+2\right)}{2\Gamma\left(2\sqrt{B_3}+n+1\right)\Gamma\left(2\sqrt{B_3+B_2+B_1}+n+2\right)}\right]^{\frac{1}{2}}. \tag{24}$$

3. PERCENTAGE DEVIATION AND ERROR

The absolute percentage deviation is calculated using Eq. (28)

$$\sigma=\frac{100}{M}\sum\left|\frac{T_v-T_{RKR}}{T_{RKR}}\right|, \tag{28}$$

where T_{RKR} is the experimental data, T_v is the present results and M is the number of experimental data [40].

The percentage error is computed with Eq. (29)

$$err_p=\frac{\sum_v RD}{T_{RKR}}\times 100\% \tag{29}$$

4. RESULTS AND DISCUSSION

The energies for $X^1\Sigma^+$ state of ScI and $X^3\Sigma^-$ state of NI using Eq. (19), as while as the relative deviation However (RD) of the calculated results and the experimental data are given in Table 2. The experimental data is taken from [41] as shown in Table 1. We note that the energies becomes larger as the quantum state increases for the two molecules, the RD for $X^3\Sigma^-$ state of NI are higher compared to the RD for $X^1\Sigma^+$ state of ScI. We deduce that the ScI is more fitted for the calculation compared to NI. Using Eq. (28), the percentage deviation (PD) for the molecules is calculated. We note that the PD for ScI is 0.015% while that of NI is 0.021%. Also, with Eq. (29), we determine the percentage error (PE) of the present results to the experimental data, the PE of the calculated result is computed and the results shows that for ScI we have 0.12% while that of the NI is 0.21%. In Fig. 1, we plotted the energy spectra with the principal quantum number for the selected molecules. It was observed that as the principal quantum number increase the energy spectra of the molecules increases linearly.

Table 1. Molecular constants for electronic states of NI and ScI [41]

Molecule	μ	State	$\omega_e\ (cm^{-1})$	$D_e(cm^{-1})$	$\vartheta_e\ (cm^{-1})$	$r_e(\dot{A})$
NI	12.6114.	$X^3\Sigma^-$	604.70	0.3460	0.0031700	1.9653
ScI	33.1961	$X^1\Sigma^+$	277.18	0.7467	0.0002834	2.6078

Table 2. Comparison of the calculated energies (cm^{-1}) for $X^1\Sigma^+$ state of ScI and $X^3\Sigma^-$ state of NI with the experimental data

n	Present work	Scl [41]	Relative deviation (RD)	Present work	NI [41]	Relative deviation (RD)
0	138.4120	138.3	0.1120	301.2234	301.1	0.1234
1	414.7977	413.9	0.8976	897.0135	896.6	0.9135
2	688.1130	687.7	0.4130	1482.6617	1482.3	0.6617
3	960.1402	959.9	0.2402	2060.5594	2058.8	1.7594
4	1231.1101	1230.4	0.7101	2625.9124	2625.9	0.9124
5	1500.6044	1499.3	1.3044	3185.1171	3183.6	1.5171
6	1767.1278	1766.5	0.6278	3732.8788	3731.9	0.9788

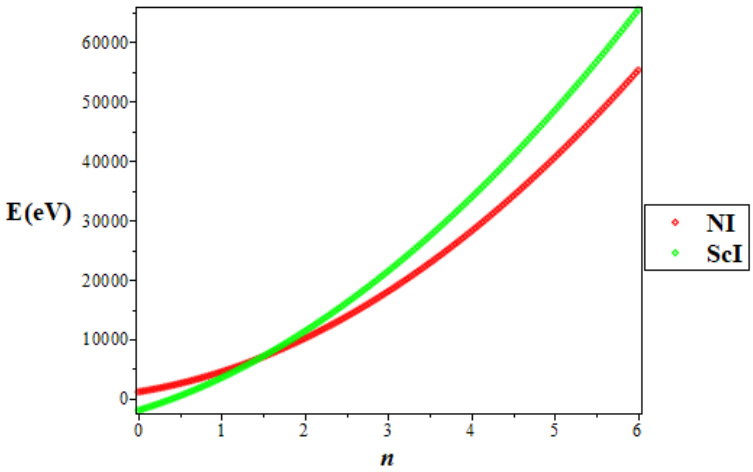

Figure 1. Variation of Energy spectra with principal quantum a number for the selected diatomic molecules

CONCLUSION

In this research, the SE with the SKP is solved using the NU method. The energy spectrum and the wave function were obtained with the Greene-Aldrich approximation to the centrifugal barrier. We then applied the energy spectrum to calculate the energies of ScI and NI molecules. The results agreed excellently with the experimental data of the two molecules. The PD shows that the SKP is fitted in the calculation of ScI than NI since the PD in ScI is lesser than that of NI molecule. This research finds application in chemistry, industry, molecular physics and studies on magnetocaloric effect for several molecules. Our findings also demonstrate that the approximation scheme is well suited for this potential.

Funding. N/A
Conflicts of interest/Competing interests. The authors declare no competing interests.
Authors' contributions. Dr. Etido P. Inyang suggested the point research and the writing of the full manuscript and Dr. Effiong O. Obisung proofread the manuscript.

ORCID ID

Etido P. Inyang, https://orcid.org/0000-0002-5031-3297

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ДОСЛІДЖЕННЯ ЕЛЕКТРОННИХ СТАНІВ МОЛЕКУЛ NI ТА ScI З ЕКРАНОВАНИМ ПОТЕНЦІАЛОМ КРАТЦЕРА

Етідо П. Ін'янг[a], Ефйонг О. Обісунг[b]

[a]*Фізичний факультет, Національний відкритий університет Нігерії, Джабі, Абуджа, Нігерія*

[b]*Фізичний факультет, Калабарський університет, Калабар, Нігерія*

У цьому дослідженні за допомогою відомого методу Нікіфорова-Уварова аналітично розв'язується рівняння Шредінгера з екранованою потенціальною моделлю Кратцера. Отримано енергетичний спектр і нормовану хвильову функцію з наближенням Гріна-Олдріча для відцентрового члена. Енергетичний спектр використовується для генерації власних значень для $X^3\Sigma^-$ стану NI та $X^1\Sigma^+$ стану молекул ScI відповідно. Розрахункові результати добре узгоджуються з експериментальними даними. Це дослідження знайшло застосування в хімії, промисловості, молекулярній фізиці та дослідженнях магнітокалоричного ефекту для кількох молекул. Наші результати також демонструють, що схема апроксимації добре підходить для цього потенціалу.

Ключові слова: рівняння Шредінгера; метод Нікіфорова-Уварова; екранований потенціал Кратцера; молекули