Research article

Eigen-solutions and thermal properties of multi-parameter exponential potential

C.A. Onate a,*, I.B. Okon b, M.C. Onyeaju c, E. Omugbe d, A.D. Antia b, J.P. Araujo e, Chen Wen-Li f

a Department of Physical Sciences, Redeemer’s University, Ede, Nigeria
b Theoretical Physics Group, Department of Physics, University of Uyo, Nigeria
c Department of Physics, University of Port Harcourt, Choba, Nigeria
d Department of Physics, Federal University of Petroleum Resources, Effurun, Nigeria
e Theoretical Physics Group, Department of Physics, University of Uyo, Nigeria
f School of Intelligent Science and Information Engineering, Xi’an Peihua University, Xi’an, 710125, China

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ABSTRACT

In this work, we determined an approximate eigen solutions of Modified multi-parameter exponential potential using supersymmetric quantum mechanics approach (SUSY) with improved Greene-Aldrich approximation to the centrifugal term. The energy equation and its corresponding normalised radial wave function were fully obtained. The proposed potential reduces to other useful potentials like Rosen-Morse, Hellmann, Yukawa and Coulomb potential as special cases. The thermodynamic properties like the vibrational mean energy \( \langle U(\beta, V) \rangle \), Vibrational heat capacity \( \langle C(\beta, V) \rangle \), vibrational entropy \( \langle S(\beta, V) \rangle \) and vibrational free energy \( \langle F(\beta, V) \rangle \) of the interacting potential were studied via partition function \( \langle Z(\beta, V) \rangle \) obtained from the resulting energy equation. This study was applied to three diatomic molecules: Chromium hydride (CrH), Titanium Hydride (TiH) and Thiocynate (SCN). To ascertain the high degree of our analytical mathematical accuracy, we compared the results of special cases with an existing results. These were found to be in excellent agreement with the existing results.

1. Introduction

Because of their numerous applications in chemical, physical, and molecular spectroscopy, many diatomic molecular potentials have been used to study bound state solutions of both relativistic and non-relativistic wave equations. Meanwhile, a thorough understanding of molecular structure is dependent on the atom’s inter-nuclear interactions and the molecular potential model under consideration [1]. The Deng-Fan potential [2], Tietz-Wei potential model [3], Improved deformed four parameter exponential potential [4], Tietz-Hua potential [5, 6, 7], Morse and Modified Morse potential [8], Deng-Fan-Eckart potential [9], Molecular attractive potential model [10], Mobius square plus Screened Kratzer potential [10], Four parameter potential [11], Varshni potential [12, 13], New generalized Morse-like potential exists in various forms in all of these potential models. The various forms of the Morse potential, on the other hand, have been used to investigate the physical behavior of semiconductor surfaces and interfaces [14, 15, 16]. The Morse potential has been successfully used to model hydrogen bonds connecting two bases in a pair in the study of thermal denaturation of double DNA, stranded-DNA chains [16, 19, 20, 21, 22]. Morse potential is a better diatomic potential model for describing potential energy than other diatomic potential models. A great deal of research has been done on Morse and other exponential-type potentials. Pena et al. [23], for example, investigated the D-dimensional Schrödinger equation for a class of multi-parameter exponential type potentials, they obtained eigenfunctions and eigenvalues for Mie-Type, Coulomb, and Kratzer-Fues potentials as special cases. Okorie et al. [24] investigated the thermodynamic properties of the improved deformed exponential-type potential (IDEP) for some diatomic systems, they obtained the ro-vibrational energy spectra of the potential model using coordinate transformation and the Greene-Aldrich approximation to centrifugal term. Omugbe et al. [11] investigated the unified treatment of non-relativistic bound state solutions, thermodynamic properties, and expectation values of exponential type potentials within the framework of the semi-classical WKB approach. On a general ground several studies have been reported on the Schrödinger equation for some potentials [25, 26, 27, 28]. The rotational Morse potential as a function of bond length was calculated by Theaban and Wadi [29]. The electronic state of the lithium molecule was

* Corresponding author.
E-mail address: oaclems14@physicist.net (C.A. Onate).

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### Table 1. Spectroscopic constants for the selected diatomic molecules.

| Molecules | $D_0$(eV) | $r_a$(Å) | $\lambda(\text{amu})$ | $\mu$(amu) |
|-----------|------------|----------|------------------------|------------|
| CrH       | 2.13       | 1.694    | 1.52179                | 0.988076   |
| TiH       | 2.05       | 1.781    | 1.32408                | 0.987371   |
| ScN       | 4.56       | 1.768    | 1.50680                | 10.628771  |

### Table 2. Bound state energies for CrH, TiH and ScN diatomic molecules for the multi-parameter exponential potential for $(\alpha, \alpha_1, \alpha_2 = 1)$. 

| n | $E_n$(eV) | $E_n$(eV) | $E_n$(eV) |
|---|----------|----------|----------|
|   | CrH      | TiH      | ScN      |
| 0 | 0.001    | -2.36945 | -2.38925 |
| 1 | 0.001    | -4.73891 | -4.75871 |
| 2 | 0.001    | -7.10836 | -7.12816 |
| 3 | 0.001    | -9.47831 | -9.49811 |
| 4 | 0.001    | -11.84826| -11.86806|
| 5 | 0.001    | -14.21821| -14.23801|

### Table 3. Bound state energies $-E_n$(eV) for CrH, TiH and ScN diatomic molecules for the multi-parameter exponential potential for $(\alpha, \alpha_1, \alpha_2 = -1)$. 

| n | $E_n$(eV) | $E_n$(eV) | $E_n$(eV) |
|---|----------|----------|----------|
|   | CrH      | TiH      | ScN      |
| 0 | 0.001    | 2.36945  | 2.38925  |
| 1 | 0.001    | 4.73891  | 4.75871  |
| 2 | 0.001    | 7.10836  | 7.12816  |
| 3 | 0.001    | 9.47831  | 9.49811  |
| 4 | 0.001    | 11.84826 | 11.86806 |
| 5 | 0.001    | 14.21821 | 14.23801 |

### Table 4. Comparison of Eigenvalues ($-E_n$) in atomic units for the Hellmann potential and Coulomb potential.

| State | Present | NU [39] | PTB [40] | Present | NU [39] | AP [39] |
|-------|---------|---------|---------|---------|---------|---------|
| $1s$  | 2.249500| 2.249500| 2.249000| 2.248500| 2.248500| 2.247000|
| $2s$  | 2.247506| 2.252506| 2.255010| 2.252506| 2.252506| 2.233057|
| $3p$  | 2.246502| 2.252502| 2.255010| 2.252506| 2.252506| 2.233057|

### 2. Radial solution of Schrödinger equation using supersymmetric quantum mechanics approach (SUSY)

The bound state solutions for the proposed potential is obtained in this section. The radial Schrödinger equation as

$$\frac{\hbar^2}{2\mu} \frac{d^2 R_n(r)}{dr^2} + V(r)R_n(r) + \frac{\hbar^2}{2\mu} \frac{\ell(\ell + 1)}{r^2} R_n(r) = E_n R_n(r),$$

where the energy of the is $E_n\ell$, $\hbar$ is Planck's constant, $\mu$ is the reduced mass, $R_n(r)$ is the wave function and $V(r)$ is the interacting potential given by

$$V(r) = D_0 + a_0 \lambda + a_2 \lambda^2 + \frac{a_4 \lambda^4 + a_6 \lambda^2 e^{i\phi}}{1 - e^{-i\phi}} + \frac{a_8 + a_6 e^{2i\phi}}{(1 - e^{-i\phi})^2 \phi^2}.$$

The centrifugal term in Eq. (1) can be approximated by the formula [33].

$$\frac{\lambda^2}{2\mu} \frac{1}{(1 - e^{-i\phi})^2 \phi^2} \approx \frac{\lambda^2}{\phi^2}$$
To solve equation in Eq. (1) using supersymmetric approach, Eq. (2) and Eq. (3) are first substituted into Eq. (1) to have

\[
\frac{d^2 R_{\alpha \ell}(r)}{dr^2} = \left[ V_p + \frac{2a_{\alpha} \lambda}{\lambda + \rho_0} + V_F e^{-2i\rho} - \ell(\ell + 1) \frac{\lambda^2 e^{-i\rho}}{(1 - e^{-i\rho})^2} \right] R_{\alpha \ell}(r),
\]

where

\[
V_p = \ell(\ell + 1) a^2 + \frac{2\mu (a D_x + a_0 D_y - E_{\alpha \ell})}{\hbar^2},
\]

\[
V_F = \frac{2\mu D_x (a_2 + a_0 e^{i\rho})}{\hbar^2} - \ell(\ell + 1) a^2,
\]

\[
V_R = \frac{2\mu D_x (a_2 + a_0 e^{i\rho})}{\hbar^2}.
\]

Eq. (5), Eq. (6) and Eq. (7), are used for simplicity. The use of supersymmetric approach involves the proposition of superpotential function as a general solution to Riccati equation. Thereafter, the supersymmetric partner potential can be constructed where a simple mapping of the desire result is formed to determine the energy equation [34, 35, 36]. To proceed from Eq. (4), first the ground state wave function is written as

\[
R_{\alpha \ell}(r) = \exp \left( - \int W(r) dr \right),
\]

Where \(W(r)\) is called superpotential function in supersymmetric quantum mechanics. The ground state wave function corresponds to the two partner Hamiltonians [37].

\[
H_+ = \tilde{A} \tilde{A}^\dagger = -\frac{d^2}{dr^2} + V_+(r),
\]

\[
H_- = \tilde{A} \tilde{A}^\dagger = -\frac{d^2}{dr^2} + V_-(r),
\]

where

\[
\tilde{A} = -\frac{d}{dr} - W(r),
\]

\[
\tilde{A} = \frac{d}{dr} - W(r).
\]

Substituting Eq. (8) into Eq. (4) leads to a non-linear Riccati equation of the form

\[
W^2(r) - \frac{dW(r)}{dr} = V_p + \frac{2a_{\alpha} \lambda}{\lambda + \rho_0} + V_F e^{-2i\rho} - \ell(\ell + 1) \frac{\lambda^2 e^{-i\rho}}{(1 - e^{-i\rho})^2},
\]

To proceed from Eq. (13), we propose a superpotential function of the form

\[
W(r) = \rho_0 + \frac{\rho_1}{1 - e^{-i\rho}}.
\]

and substituting it into Eq. (13) with the consideration that the radial wave equation satisfy the boundary conditions that \(R_{\alpha \ell}(r)/r\) becomes zero as \(r \to \infty\), and \(R_{\alpha \ell}(r)/r\) is finite when \(r = 0\), some simple mathematical manipulations and simplifications result to the following equations

\[
\rho_0^2 = V_p,
\]

\[
\rho_1 = \frac{\lambda \pm \sqrt{\lambda^2 + 4\ell(\ell + 1) a^2 + 4V_0 a^2}}{2}
\]

\[
\rho_0 = \frac{V_p + V_F - \frac{2a_{\alpha} \lambda}{\lambda + \rho_0}}{2\rho_1} - \rho_1.
\]

Eq. (15), Eq. (16) and Eq. (17) are the bases for the energy equation. Using Eq. (14) in conjunction with Eqs. (9), (10), (11), and (12), the two partner potentials of the supersymmetry quantum mechanics can fully be written in the form.
subsequently, the recurrence relation is generalized as

\[ R(n) = \frac{\psi'(n)}{\psi(n)} \]

\[ R(n+1) = \frac{\psi'(n+1)}{\psi(n+1)} \]

It can be seen from Eq. (18) and Eq. (19) that the family potentials satisfied a shape invariance condition which established a relation of the form

\[ V_1(a_0, r) = V_2(a_1, r) + R(a_1), \]

via mapping of the form \( \rho_1 \to \rho_1 + \lambda \), where \( \rho_1 = a_0 \). In terms of the parameters of the partner potentials in Eq. (20), the relation \( a_1 = f(a_0) = a_0 + n \), where \( a_1 \) is a new set of parameters uniquely determined from an old set of parameters \( a_0 \), the term \( R(a_1) \), is called a remainder or residual term and it is independent of the variable \( r \). Since \( a_1 = a_0 + \lambda \), then, \( a_2 = a_0 + 2\lambda \), \( a_3 = a_0 + 3\lambda \), \( a_4 = a_0 + 4\lambda \), subsequently, the recurrence relation is generalized as \( a_n = a_0 + n\lambda \). Using the shape invariance approach \([37]\), the recurrence relations above, Eq. (20) is transformed as

\[ R(a_1) = \left( \frac{V_R + V_I - \frac{2a_1}{r^2} - a_1^2}{2a_0} \right)^2 - \left( \frac{V_R + V_I - \frac{2a_2}{r^2} - a_2^2}{2a_1} \right)^2, \]

\[ R(a_2) = \left( \frac{V_R + V_I - \frac{2a_2}{r^2} - a_2^2}{2a_1} \right)^2 - \left( \frac{V_R + V_I - \frac{2a_3}{r^2} - a_3^2}{2a_2} \right)^2, \]

\[ R(a_3) = \left( \frac{V_R + V_I - \frac{2a_3}{r^2} - a_3^2}{2a_2} \right)^2 - \left( \frac{V_R + V_I - \frac{2a_4}{r^2} - a_4^2}{2a_3} \right)^2, \]

\[ R(a_4) = \left( \frac{V_R + V_I - \frac{2a_4}{r^2} - a_4^2}{2a_3} \right)^2 - \left( \frac{V_R + V_I - \frac{2a_5}{r^2} - a_5^2}{2a_4} \right)^2. \]

Using the negative partner potential, the energy equation of the system can be written as

\[ E_{a_0} = \sum_{k=1}^n \frac{2}{2a_0} \left( \frac{V_R + V_I - \frac{2a_0}{r^2} - a_0^2}{2a_0} \right)^2, \]

which on correct substitution of the parameters of the system into Eq. (25) using Eqs. (15), (16), and (17) and Eqs. (21), (22), (23), and (24) gives a complete energy equation in a one-dimensional system as

\[ E_{a_0} = D_e \left( a + a_0 \lambda + a_1 \right) + \frac{\lambda^2}{2\mu} \left[ \ell \left( \ell + 1 \right) - \frac{\lambda^2}{2n + 1 + \delta_0} \left( \frac{2n + 1}{4} \right)^2 \right]. \]

\[ \delta_0 = \sqrt{1 + 2\lambda^2 + \frac{8nD_e}{\lambda^2}} \]

\[ \beta_0 = a_0 + \lambda(a_3 - a_1) \]

\[ \beta_1 = e^{\pi i} (a_4 + a_5 e^{\pi i}) \]

where Eq. (27), Eq. (28) and Eq. (29) are used for simplicity.

2.1 Special cases

The proposed potential model given in Eq. (2) can be reduced to some potential models by varying the potential parameters.

(a) Improved Rosen-Morse-like Potential \([38]\).

Substituting \( a_0 = a_1 = a_2 = 0 \), into Eq. (26) gives the energy of Improved Rosen-Morse-like potential as
Using the constant $a = a_1 = a_2 = a_3 = a_4 = a_5 = a_6 = 0$, Eq. (33) can further be reduced to

Figure 3. Wave function and probability density plots for $l = 0$ (a–b) and $l = 1$ (c–d).
The total wave function for the proposed potential is given as

\[ \psi = \beta \eta \text{ and } \eta = \frac{E_n}{\mu} \]

where \( E_n \) is the energy level of the system. Eq. (36) and Eq. (37) are used as

\[ \ell = \frac{\beta^2 r^2}{2\mu} \]

Eq. (30), Eq. (31), Eq. (32), Eq. (33) and Eq. (34) are special cases of

The wave function is assumed to be in bound at

\[ r \quad \text{is the hypergeometric function.} \]

\[ \beta = \sqrt{\frac{\ell^2 (\ell + 1) + 2\mu D(n + \alpha, b, \alpha, \beta)}{\lambda^2 \hbar^2}} \]

and \( F \) is the hypergeometric function. Eq. (36) and Eq. (37) are used as

\[ \int_0^\infty |R_n(r)|^2 \, dr = 1 \Rightarrow \int_0^\infty [N_n \alpha^2 (1 - y)^\alpha \left( I_{2(\beta - 1)}(1 - 2y) \right)^2] \, dy = 1 \]

The wave function is assumed to be in bound at \( r \in (0, \infty) \) and \( y = e^{-\beta r} \in (1, 0) \).

Figure 4. Wave function and probability density plots for \( l = 2 \) (a-b) and \( l = 3 \) (c-d).

\[ E_n = D_{a, b} \beta^2 \frac{\hbar^2}{2\mu} \left[ \ell (\ell + 1) - D_{b, c} \left( \frac{\ell^2 (\ell + 1) - (1 + n + \ell)}{2(1 + n + \ell)} \right) \right] \]  

(34)

\[ \frac{N_n^2}{2^\alpha} \int_{-1}^1 \left( \frac{1-w}{2} \right)^{-2\alpha-1} \left( \frac{1+w}{2} \right)^{2\alpha} [P_n^{(2\beta-1)}(w)]^2 \, dw = 1 \]  

(39)

Let \( z = (1 - 2y) \) such that the boundary of integration of Eq. (39) changes from \( y \in (1, 0) \) to \( z \in (-1, 1) \). Then Eq. (39) reduces to

\[ \frac{N_n^2}{2^\alpha} \int_{-1}^1 \left( \frac{1-w}{2} \right)^{-2\alpha-1} \left( \frac{1+w}{2} \right)^{2\alpha} [P_n^{(2\beta-1)}(z)]^2 \, dz = 1 \]  

(40)

Using the standard integral [31]

\[ \frac{1}{n!} \Gamma(x+n+1) \Gamma(y+n+1) \]

where we assume that \( z = w, x = 2\beta - 1, y = 2\eta \). Then, using equation (40) and Eq. (41), the normalization constant can be obtained as

\[ N_n = \sqrt{\frac{2\lambda}{\alpha} \Gamma(x+y+n+1) \Gamma(x+y+2n+1)} \]  

(41)

Using Eq. (42), the total normalized wave function is given as
Eq. (43) is a complete normalized radial wave function of the system.

3. Thermodynamic properties for the modified four parameter Morse potential

The thermodynamic properties of quantum systems can be obtained from the exact partition function given by

$$Z(\beta) = \sum_{n=0}^{\infty} e^{-\beta E_n}$$  \hspace{1cm} (44)

where, \(V\) is an upper bound of the vibrational quantum number obtained from the numerical solution of \(\frac{dE_n}{dn} = 0\), \(\beta = \frac{1}{kT}\) where \(k\) and \(T\) are Boltzmann constant and absolute temperature respectively. In the classical limit, the summation in Eq. (44) can be replaced with an integral:

$$Z(\beta) = \int_0^V e^{-\beta E_n} dn.$$  \hspace{1cm} (45)

Eq. (45) is the equation for partition function. The energy Eq. (26) can be simplified further as

$$E_{el} = v_1 - v_2 \left( \frac{v_3}{n+\delta} - (n+\delta) \right)^2.$$  \hspace{1cm} (46)
where
\[ \nu_1 = D(\theta a_0 + a_1) + \frac{\hbar^2 \lambda^2 (l + 1)}{2 \mu} ; \quad \nu_2 = 2\mu D_a(\beta \theta_0 + \beta \lambda) - l(l + 1), \]
\[ \nu_3 = \frac{\hbar^2 \lambda^2}{8 \rho} ; \quad \delta = \frac{1}{2} \sqrt{\left(1 + 2l\right)^2 + \frac{8\mu D_a(\theta a_0 + a_1 e^{z_0})}{\hbar^2 \lambda^2}}. \]

Let \( \rho = (n + \delta) \), then Eq. (46) can then be express as
\[ E_n = - \left[ \nu_2 \rho^2 + \frac{\nu_3 \rho^2}{\rho^2} \right] + \nu_1 - 2\nu_2 \nu_3 \]

Using Eq. (47) and Eq. (48), the partition function of Eq. (26) can then be express as
\[ Z(\beta) = e^{\beta(2\nu_3 - \nu_1)} \int_0^\rho e^{-\left[ \nu_2 \rho^2 + \frac{\nu_3 \rho^2}{\rho^2} \right]} d\rho \]

Using Mathematica 10.0 version, the partition function of Eq. (49) is obtained as
\[ Z(\beta) = \frac{\left[e^{\beta(\gamma_2(1 + \chi_4) + e^{\beta(\gamma_2)}(-1 + \chi_5)}\right]}{4\sqrt{-\beta_0^2}} \]

where
\[ \chi_1 = \beta(-\nu_1 + 2\nu_2 \nu_3), \quad \chi_2 = 2 \sqrt{-\beta_0^2 \sqrt{-\beta_0^2 \nu_3^2}}, \quad \chi_3 = -2 \sqrt{-\beta_0^2 \sqrt{-\beta_0^2 \nu^2_3}}, \quad \chi_4 = \text{erf} \left[ \frac{\nu \sqrt{-\beta_0^2 - \sqrt{-\beta_0^2 \nu_3^2}}}{V} \right], \quad \chi_5 = \text{erf} \left[ \frac{\lambda \sqrt{-\beta_0^2 + \sqrt{-\beta_0^2 \nu_3^2}}}{V} \right]. \]

Eq. (50) gives the complete partition function while Eq. (51) is used for simplicity.
(a) Vibrational mean energy

\[ U(\beta) = -\frac{\partial \ln Z(\beta)}{\partial \beta} = U(\beta) = \right\]

\[ -\left\{ \frac{1 + \chi_4 + e^{2\chi_2}(\chi_3 - 1) - 2\beta [1 + \chi_4 + e^{2\chi_2}(\chi_3 - 1)]w_0 + \alpha_4 \sqrt{-\beta \omega_2} \sqrt{\pi \beta} (-1 - e^{2\chi_2} - \chi_4 + e^{2\chi_2} \chi_3) \omega_3^2 - e^{2\chi_2} \omega_2^2 }{2\beta [1 + \chi_4 + e^{2\chi_2}(-1 + \chi_3)]} \right\} \]

(52)

where

\[ w_0 = (-\omega_1 + 2\omega_3) \quad w_1 = \frac{1}{\sqrt{\pi \beta} \sqrt{-\beta \omega_2 \omega_3^2} \omega_2} \quad w_2 = \frac{\beta \omega_2 (\chi_4 + \omega_3^2)}{\chi_3 - \sqrt{-\beta \omega_2 \omega_3^2}} \]

(53)

Eq. (52) is a vibrational mean energy while Eq. (53) are used for simplicity.
(b) Vibrational Specific heat capacity

\[ C(\beta) = K \frac{\beta^2 \ln Z(\beta)}{\beta^2} \]

\[ = \frac{\left\{ \pi \lambda \left( 1 - e^{2\beta_3 \lambda V + e^{2\beta_3 \lambda X_3}} \right)^2 \omega_3 + \Phi_0 + \Phi_1 + \Phi_2 - 8e^{2\beta_3 \lambda V \omega_3} + \Phi_3 + \Phi_4 \right\}}{2\pi \lambda \left( 1 - e^{2\beta_3 \lambda V + e^{2\beta_3 \lambda X_3}} \right)^2 \omega_3} \]

where

\[ \Phi_0 = 2e^{2\beta_3 \lambda V \omega_3} \beta \lambda^2 \omega_3 \left[ \sqrt{\pi} - e^{2\beta_3 \lambda V + e^{2\beta_3 \lambda X_3}} \right] \omega_3, \Phi_1 = 4e^{2\beta_3 \lambda V \omega_3} \left[ - e^{2\beta_3 \lambda V + e^{2\beta_3 \lambda X_3}} \right] \omega_3, \Phi_2 = 8e^{2\beta_3 \lambda V \omega_3} \left[ - 4\beta \lambda^2 \sqrt{\omega_3 \omega_2} + \sqrt{-\beta \omega_2 \omega_2^3} \right], \]

\[ \Phi_3 = e^{2\beta_3 \lambda V \omega_3} \left[ 8\sqrt{\pi} \lambda \omega_3 + \omega_3^2 \left[ - 4\beta \lambda^2 \sqrt{\omega_3 \omega_2} + \sqrt{-\beta \omega_2 \omega_2^3} \right] \right], \]

\[ \Phi_4 = \left[ - 8e^{2\beta_3 \lambda V \omega_3} \sqrt{\pi} \lambda \omega_3 + 8e^{2\beta_3 \lambda V \omega_3} \omega_3^2 \right], \omega_3 = \sqrt{-\beta \omega_2 \omega_2^3}, \omega_4 = \frac{\beta \omega_2^2 (V^4 + \nu_3^2)}{V^2}, \]

\[ \omega_5 = V^2 \sqrt{-\beta \omega_2 \omega_2^3}, \omega_6 = \sqrt{-\beta \omega_2 \omega_2^3} \]

Figure 8. Variation of U(\lambda) against \lambda for CrH (a), TiH (b) and ScN (c).

Eq. (54) is a vibrational specific heat capacity while Eq. (55) is used for simplicity.
Eq. (56) is a vibrational entropy.

\[
S(\beta) = k \ln Z(\beta) - k \beta \ln Z(\beta) = k \ln \left[ \frac{e^{\beta \omega_0 + 2\beta \omega_0 - \beta^2} \sqrt{\omega_0} \left[ 1 + \chi_4 + e^{\beta \omega_0} (\chi_5 + 1) \right]}{4 \sqrt{-\beta \omega_0}} \right]
\]

\[
- K \beta \left\{ \frac{1 + \chi_4 + e^{\beta \omega_0} (\chi_5 - 1) - 2\beta (1 + \chi_4 + e^{\beta \omega_0} (\chi_5 + 1))\omega_0}{4 \sqrt{-\beta \omega_0} (\sqrt{\omega_0} \beta (e^{\beta \omega_0} (\chi_5 - e^{\beta \omega_0} - \chi_4 - 1)\omega_0^2 - e^{\beta \omega_0} (\chi_5 - 1))} \right\}
\]

\[
2\beta (1 + \chi_4 + e^{\beta \omega_0} (\chi_5 - 1))
\]

(56)

Eq. (56) is a vibrational entropy.

(d) Vibrational free energy

\[
F(\beta) = - \frac{1}{\beta} \ln Z(\beta) = - \frac{e^{\beta \omega_0} \ln \sqrt{\omega_0} (e^{\beta \omega_0} (\chi_4 + 1) + e^{\beta \omega_0} (\chi_5 - 1))}{4 \sqrt{-\beta \omega_0}}
\]

(57)

Eq. (57) is a vibrational free energy

4. Results and discussion

Table 1 shows the standard spectroscopic parameters for all the diatomic molecules used in this work. Tables 2 and 3 are the numerical bound state energies computed using Eq. (26), the spectroscopic constants of Table 1 and the arbitrary constants \((a, a_1, \ldots, a_6 = 1.0)\) and \((a, a_1, \ldots, a_6 = -1.0)\) for CrH, TiH and ScN molecules respectively. From Tables 2 and 3, the numerical bound state solutions of these molecules decreases with an increase in quantum state but increases with an increase in the angular momentum quantum state. Table 4 are the numerical solutions of Hellmann potential and Coulomb potential as special cases of the potential in the present work. The results of the special cases in Table 4 were also compared with an existing literature. The numerical solutions as reported in this table are in excellent agreement with the reports of other researchers.

Figure 1 (a) shows the potential for the present study. Figure 1(b) shows the approximation scheme. Figure 2 is the variation of bound state energy spectral with screening parameter \(\lambda\) and dissociation energy \(D_e\) (is presented). The variation of spectral in Figure 2 shows unique quantisation of different energy level. Figures 3(a-d) shows the wave function
and probability density for orbital angular quantum number \( l = 0 \) and \( l = 1 \) respectively. While Figures 4 (a-d) are the wave function plots and probability density plots for orbital angular quantum number \( l = 2 \) and \( l = 3 \) respectively. Both Figures 3(a-d) and 4(a-d) reproduces similar trend as reported in other literatures.

In Figure 5 and Figure 6, we examined the how the vibrational partition function varies with the temperature parameter and maximum quantum state for CrH, TiH and ScN. In Figure 5, the partition function and the temperature varies inversely with each other for the three diatomic molecular systems. At absolute zero, the partition function at various maximum quantum state tends to converged but diverged as the temperature decreases. In Figure 6, the partition function increases as the maximum quantum state increases for TiH and ScN. However, for CrH, the partition function decreases for \( \beta = 0.00000102, 0.00000103 \) and 0.00000104 but increases for \( \beta = 0.00000105 \) as the maximum quantum state increases. The behaviour of partition function against V for TiH and ScN are similar while that of CrH differs.

The variation of the vibrational mean energy against the temperature parameter and maximum quantum state respectively for CrH, TiH and ScN are shown in Figures 7 and 8. In Figure 7, the vibrational mean energy decreases monotonically as the temperature of the system decreases gradually for all the molecules. The vibrational mean energy at various V are the same for three molecules at all values of \( \beta \). Although, the mean energy for the three molecules exhibit the same features but that of the ScN has lower values compared to CrH and TiH. In Figure 8, the vibrational mean energy increases as the maximum quantum state increases for TiH. However, for CrH, the vibrational mean energy decreases for the first \( \beta = 0.00000102, 0.00000103 \) and 0.00000104 and the mean energy are found to be greater than zero but for \( \beta = 0.00000105 \), the mean energy increases as V increases. The mean for the last value of \( \beta \)
Figure 11. Variation $S(\beta)$ against $\beta$ for CrH (a), TiH (b) and ScN (c).
even when it increases is seen to be less than zero. The behaviour of the mean energy against V for ScN is opposite to that of the CrH.

The variation of the vibrational specific heat against the temperature parameter and maximum quantum state for CrH, TiH and ScN are shown in Figures 9 and 10 respectively. In Figure 9, the specific heat capacity rises significantly as the temperature parameter increases for all the molecules. The specific heat capacity at different values of V tends to converge as the specific heat capacity is almost zero. In Figure 10, though the specific heat capacity rises as the maximum quantum state increases for all molecules, but the variation in CrH and TiH are the same while that of ScN differs. In Figures 10 (a) and (b), the specific heat capacity for various β converges when the specific heat capacity is zero after which they diverged as the rise significantly.

In Figures 11 and 12, we plotted the vibrational entropy against the temperature parameter and maximum quantum state for CrH, TiH and ScN. The vibrational entropy increases while the temperature parameter increases for the three molecules considered in this work. The vibrational entropy for various maximum quantum state diverges as they increase from zero. In Figure 12, the vibrational entropy for TiH and ScN decreases and have a turning point as the maximum quantum state increases steadily. The turning point for the two molecules are not very far from each other. For CrH, the vibrational entropy decreases as the maximum quantum state increases.

The variation of the vibrational free energy against the temperature parameter and the maximum quantum state for CrH, TiH and ScN are shown in Figures 13 and 14 respectively. The vibrational free energy for
all maximum quantum state decreases monotonically as the temperature parameter increases gradually for the three molecules in Figure 13. However, the vibrational free energy for various $V$ for ScN converged when the $\beta$ is zero and diverged as $\beta$ gradually increases. This particular feature is not observed in CrH and TiH. In Figure 14, CrH and ScN have the same variation while that of TiH differs. The vibrational free energy increases as $V$ increases for CrH and ScN, though the increase terms to be insignificant for $V$ ranges from 0 to about 3 and a sharp increase is noticed but the vibrational free energy of TiH decreases as $V$ increases for some values before it begins to have a turning point. The thermal properties are useful in different scientific fields e.g. regulation of heat content.

## 5. Conclusion

In this research work we calculated an approximate bound state solutions of four parameter Morse potential using supersymmetric quantum mechanics approach. The energy eigen equation is presented in a closed form and extended to study partition function and other thermodynamic properties for three diatomic molecules using standard spectroscopic constants. The proposed potential reduces to Improved Rosen Morse, Hellmann, Yukawa and Coulomb potential as special cases. The numerical bound state solutions obtained for some of the special cases are in excellent agreement with an existing literature. The normalised wave function and probability density plots were obtained for various quantum
state and orbital angular quantum number. The thermal properties for the three molecules studied in some cases showed the same characteristics while in some areas, their thermal properties exhibit different features. The results obtained are applicable in Molecular Physics especially in the field of spectroscopy.

**Declarations**

**Author contribution statement**

C.A. Onate: Conceived and designed the experiments; Analyzed and interpreted the data; Wrote the paper.

I.B. Okon: Conceived and designed the experiments; Performed the experiments; Wrote the paper.

E. Omugbe, A.D. Antia: Performed the experiments; Wrote the paper.

M.C. Onyeaju: Analyzed and interpreted the data; Wrote the paper.

J.P. Araujo, Chen Wen-Li: Contributed reagents, materials, analysis tools or data; Wrote the paper.

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**Declaration of interest’s statement**

The authors declare no conflict of interest.
