Determination of thermodynamic properties of *CrH*, *NiC* and *CuLi* diatomic molecules with the linear combination of Hulthen-type potential plus Yukawa potential

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ABSTRACT

In this work, we investigate the thermodynamic properties of *CrH*, *NiC* and *CuLi* diatomic molecules with a linear combination Hulthen and Yukawa potentials in the presence and absence of magnetic and Aharanov-Bohm (AB) fields. The Schrödinger equation in 3D and 2D were solved using the Nikiforov-Uvarov (NU) method and the exact quantization rule (EQR) respectively. To determine the thermodynamic properties for the selected diatomic molecules, we first used the energy spectrum to evaluate the partition function and other thermodynamic functions such as entropy, Helmholtz free energy, internal energy and specific heat capacity. In addition, it is found that in the classical limit, the specific heat capacity saturates for large values of the principal quantum number, $n_{\max}$ for the selected diatomic molecules at a fixed temperature except *CrH*. Our results can be applied to molecular physics and chemical physics.

1. Introduction

The exact solution of the Schrödinger equation (SE) with a chosen potential model is fundamental for understanding the energy spectrum of a particle and also gives a complete description of the quantum mechanical system in consideration [1,2]. The exact solution of Schrödinger wave equation is only possible for a few potentials such as harmonic oscillator potential, Coulomb potential, Kratzer, etc. Different methods such as the modified factorization method [3,4], asymptotic iteration method [5,6], Nikiforov-Uvarov functional analysis (NUFA) method [7], Nikiforov-Uvarov method (NU) [8], and others have been employed to solve non-relativistic wave equations. The Nikiforov-Uvarov is an analytical method based on the solution of the second-order linear differential equations with special orthogonal function [8]. This method transforms the Schrödinger equation in

spherical coordinates into a generalized geometric-type differential equation with an appropriate coordinate transformation $r \rightarrow s$. The NU method provides an exact solution to the spherical SE simpler, more elegant, and direct as compared to other traditional methods [8]. In this particular study, we considered the linear combination of the Hulthen and Yukawa potentials. The Hulthen potential which has a Coulombic attractive behavior for small r has the form [9,10]

$$V_H(r) = -\frac{V_0 e^{-2\delta r}}{1 - e^{-2\delta r}} \tag{1.1}$$

where $V_0 = Ze^2\delta$, Z is the atomic number and δ is the screening parameter. On the other hand, the Yukawa potential describes strong interaction between nucleons and has the form [11]

$$V_Y(r) = -\frac{V_0 e^{-\delta r}}{r} \tag{1.2}$$

where V_0' is the strength of the potential. These two potentials have Coulombic behavior at small r but go down exponentially for larger r. The linear combination of Hulthen and Yukawa potentials (HYP) is in the form

$$V(r) = -\frac{Ze^2 \delta e^{-2\delta r}}{1 - e^{-2\delta r}} - \frac{V_0 e^{-\delta r}}{r} \tag{1.3}$$

Recently, Dong et al. [12] solved the Klein Gordon (KG) equation with the linear combination of Hulthen and Yukawa potentials using Nikiforov-Uvarov method. Although different methods have been used to obtain bound-state solutions with these potential models, the solutions of the Schrödinger equation with the linear combination of the Hulthen and Yukawa potentials have not been reported in the literature [13–15]. The solution of the SE paves way for the calculation of the partition function $Z(\beta)$ followed by evaluation of other thermodynamic functions such as the entropy $S(\beta)$, Helmholtz free energy $F(\beta)$, internal energy $U(\beta)$, and specific heat capacity $C(\beta)$. Presently quite an effort is made for a better understanding of thermodynamic properties for diatomic molecules by several authors in molecular physics. Moreover, the importance of molecular vibration and rotational spectroscopy has extensive research fields for scientific areas such as Biology and Environmental science [16]. Ikot and his collaborators [17] studied thermodynamic functions for exponential-type molecule potentials in D-dimensions. Also, Okorie et al. [18] calculated the thermodynamic functions for *CO*, *NO*, and N_2 with the modified Kratzer plus screen coulomb potential using the modified factorization method. Recently, Ghanbari and Khordad [16] investigated theoretical thermodynamic properties for *CO* and N_2 using pseudo harmonic and Mie-type potentials and many other efforts by several researchers [17-25].

In addition, Jia and co-workers successfully predicted the thermodynamic properties for some diatomic substances by employing suitable potential models to represent the internal vibrations of diatomic molecules [26-30]. By employing the improved Tietz potential and Fu-Wang-Jia potential to represent the internal vibrations of triatomic molecules, some authors have successfully predicted the thermodynamic properties for some triatomic substances and the equilibrium constant for water gas shift reaction [31-35].

In this work, we analytically solve the Schrödinger equation with the linear combination of Hulthen and Yukawa potentials (HYP) using the Nikiforov-Uvarov method. The energy spectrum obtained is used to evaluate the partition function and thermodynamic properties for *CrH*, *NiC* and *CuLi*. The rest of the work is arranged as follows, in section 2, we present the bound-state solutions of the Schrödinger equation. Section 3, presents the thermodynamic properties calculation. The results are given and discussed in section 4 and finally, the conclusion is presented in section 5.

2. Bound state solutions

2.1. Bound-state solution of the Schrödinger equation with Hulthen-type potential plus Yukawa potential

In spherical coordinates the radial part of the Schrödinger wave equation is in the form [36-45];

$$\frac{d^2 R_{n\ell}(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left[E_{n\ell} - V(r) - \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2}\right] R_{n\ell}(r) = 0 \tag{2.1}$$

where $R_{n\ell}$ is the radial wave function, $E_{n\ell}$ is the energy spectrum, $\hbar$ is the reduced Planck's constant, μ is the reduced mass, and $\frac{\ell(\ell+1)}{r^2}$ is the centrifugal barrier, with ℓ and n being the angular momentum and principal quantum numbers, respectively [20] and $V(r)$ represents the combination of Hulthen and Yukawa potentials. By substituting Eq. (3)

into Eq. (4), we obtain

$$\frac{d^2 R_{n\ell}(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left[E_{n\ell} - \left(\frac{V_0 e^{-2\delta r}}{1 - e^{-2\delta r}} - \frac{V_0' e^{-\delta r}}{r}\right) - \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2}\right] R_{n\ell}(r) = 0 \tag{2.2}$$

To get rid of the centrifugal barrier in Eq. (2.2), we employ the Greene and Aldrich approximation scheme [31,33,36].

$$\frac{1}{r^2} \approx \frac{4\delta^2 e^{-2\delta r}}{(1 - e^{-2\delta r})^2} \tag{2.3}$$

Substituting Eq. (2.3) into Eq. (2.2), we have;

$$\frac{d^2 R_{n\ell}(r)}{dr^2} + \left[\frac{2\mu E_{n\ell}}{\hbar^2} - \frac{2\mu}{\hbar^2}\left(\frac{V_0 e^{-2\delta r}}{1 - e^{-2\delta r}} - \frac{2V_0' \delta e^{-2\delta r}}{(1 - e^{-2\delta r})}\right) - \frac{4\delta^2 \ell(\ell+1)e^{-2\delta r}}{(1 - e^{-2\delta r})^2}\right] R_{n\ell}(r) = 0 \tag{2.4}$$

By change of coordinate $s = e^{-2\delta r}$, the equation is rewritten as follows;

$$\frac{d^2 R_{n\ell}(s)}{ds^2} + \frac{(1-s)}{s(1-s)}\frac{dR_{n\ell}(s)}{ds} + \frac{1}{s^2(1-s)^2}\Big[$$
$$-(\varepsilon_{n\ell} + \breve{\alpha})s^2 + (2\varepsilon_{n\ell} + \breve{\alpha} - \gamma)s - \varepsilon_{n\ell}\Big]R_{n\ell}(s) = 0 \tag{2.5}$$

where we have used the following dimensionless notations for mathematical simplicity:

$$-\varepsilon = \frac{\mu E_{n\ell}}{2\hbar^2 \delta^2}; \breve{\alpha} = \frac{\mu V_0}{2\hbar^2 \delta^2} + \frac{\mu V_0'}{\hbar^2 \delta}; \gamma = \ell(\ell+1) \tag{2.6}$$

Comparing Eq. (A.1) and (2.5), the following parameters are defined as:

$$\widetilde{\tau} = (1-s), \sigma(s) = s(1-s) \text{ and } \widetilde{\sigma} = -(\varepsilon_{n\ell} + \breve{\alpha})s^2 + (2\varepsilon_{n\ell} + \breve{\alpha} - \gamma)s - \varepsilon_{n\ell} \tag{2.7}$$

Parameters $\widetilde{\tau}$, $\sigma(s)$, and $\widetilde{\sigma}(s)$ employed in Eq. (A.9) to obtain the function

$$\pi(s) = -\frac{s}{2} \pm \sqrt{\left(\frac{1}{4} + \varepsilon_{n\ell} + \breve{\alpha} - k\right)s^2 + (k - (2\varepsilon_{n\ell} + \breve{\alpha} - \gamma))s + \varepsilon_{n\ell}} \tag{2.8}$$

To find the expression for k, the discriminant of Eq. (2.8) is equated to zero. Thus we obtain,

$$k = \breve{\alpha} - \gamma \pm 2\sqrt{\varepsilon_{n\ell}}\sqrt{\frac{1}{4} + \gamma} \tag{2.9}$$

The substituting k in $\pi(s)$ of Eq. (2.8),

$$\pi(s) = -\frac{s}{2} \pm \left(\left(\sqrt{\frac{1}{4} + \gamma} + \sqrt{\varepsilon_{n\ell}}\right)s - \sqrt{\varepsilon_{n\ell}}\right) \tag{2.10}$$

Taking the negative value of $\pi(s)$ in Eq. (2.10) to obtain,

$$\pi'(s) = -\frac{1}{2} - \left(\sqrt{\frac{1}{4} + \gamma} + \sqrt{\varepsilon_{n\ell}}\right) \tag{2.11}$$

To obtain the polynomial $\tau(s)$, we use $\tau(s) = \widetilde{\tau}(s) + 2\pi(s)$

$$\tau(s) = 1 - 2s - 2\left(\left(\sqrt{\frac{1}{4} + \gamma} + \sqrt{\varepsilon_{n\ell}}\right)s - \sqrt{\varepsilon_{n\ell}}\right) \tag{2.12}$$

The derivative of $\tau(s)$ in Eq. (2.12),

$$\tau'(s) = -2\left(1 + \left(\sqrt{\frac{1}{4} + \gamma} + \sqrt{\varepsilon_{n\ell}}\right)\right) < 0 \tag{2.13}$$

The parameter λ is defined as,

$$\lambda = \breve{\alpha} - \gamma - 2\sqrt{\varepsilon_{n\ell}}\sqrt{\frac{1}{4} + \gamma} - \frac{1}{2} - \left(\sqrt{\frac{1}{4} + \gamma} + \sqrt{\varepsilon_{n\ell}}\right) \tag{2.14}$$

λ_n is expressed as,

$$\lambda_n = n^2 + n + 2n\sqrt{\varepsilon_{n\ell}} + 2n\sqrt{\frac{1}{4} + \gamma} \tag{2.15}$$

The eigenvalue expression holds if $\lambda = \lambda_n$.

$$\text{Hence, } \varepsilon_{n\ell} = \frac{1}{4}\left(\frac{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \gamma}\right)^2 - \tilde{\alpha}}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \gamma}\right)}\right)^2 \tag{2.16}$$

Substituting Eq. (2.6) into Eq. (2.16) and evaluating, we obtain the energy as follows:

$$E_{n\ell} = -\frac{\hbar^2\delta^2}{2\mu}\left(\frac{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \ell(\ell+1)}\right)^2 - \left(\frac{\mu V_0}{2\hbar^2\delta^2} + \frac{\mu V_0'}{\hbar^2\delta}\right)}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \ell(\ell+1)}\right)}\right)^2 \tag{2.17}$$

To calculate the radial wavefunction $\psi(s)$ in Eq. (A.2), we begin by evaluating $\varphi(s)$ by substituting $\pi(s)$ and $\sigma(s)$ in Eq. (A.4) to obtain

$$\frac{d\varphi(s)}{\varphi(s)} = \left(\frac{\sqrt{\varepsilon_{n\ell}}(1-s) - s\left(\frac{1}{2} + \sqrt{\frac{1}{4} + \ell(\ell+1)}\right)}{s(1-s)}\right)ds \tag{2.18}$$

Integrating Eq. (2.18), we obtain

$$\varphi(s) = s^{\sqrt{\varepsilon_{n\ell}}}(1-s)^{\frac{1}{2} + \sqrt{\frac{1}{4} + \ell(\ell+1)}} \tag{2.19}$$

From Eq. (A.5),

$$\frac{d\rho(s)}{\rho(s)} = \left(\frac{2\sqrt{\varepsilon_{n\ell}}(1-s) - 2s\left(\sqrt{\frac{1}{4} + \ell(\ell+1)}\right)}{s(1-s)}\right)ds \tag{2.20}$$

Integrating Eq. (2.20), we obtain

$$\rho(s) = s^{2\sqrt{\varepsilon_{n\ell}}}(1-s)^{2\sqrt{\frac{1}{4} + \ell(\ell+1)}} \tag{2.21}$$

Substituting Eq. (2.21) in Eq. (A.5), we get

$$y_n(s) = B_n(s)s^{-2\sqrt{\varepsilon_{n\ell}}}(1-s)^{-2\sqrt{\frac{1}{4} + \ell(\ell+1)}}\frac{d^n}{ds^n}\left[s^{n+2\sqrt{\varepsilon_{n\ell}}}(1-s)^{n+2\sqrt{\frac{1}{4} + \ell(\ell+1)}}\right]$$
$$= P_n^{\left(2\sqrt{\varepsilon_{n\ell}}, 2\sqrt{\frac{1}{4} + \ell(\ell+1)}\right)}(1-2s) \tag{2.22}$$

In terms of Jacobi Polynomial, the complete wave function of the of the HKP is given as,

$$R_{n\ell}(s) = B_n s^{\sqrt{\varepsilon_{n\ell}}}(1-s)^{\frac{1}{2} + \sqrt{\frac{1}{4} + \ell(\ell+1)}}P_n^{\left(2\sqrt{\varepsilon_{n\ell}}, 2\sqrt{\frac{1}{4} + \ell(\ell+1)}\right)}(1-2s) \tag{2.23}$$

2.2. Bound-state solution of the Schrödinger equation with Hulthen-type potential plus Yukawa potential with AB flux and magnetic fields

The Hamiltonian operator of a particle that is charged and subjected to move in the Hulthen-Type potential plus Yukawa potential under the combined impact of AB flux and an external magnetic fields with topological defect can be written in cylindrical coordinates. Thus, the Schrödinger equation for this consideration is written as follows [19];

$$\left[\frac{1}{2\mu}\left(i\hbar\overrightarrow{\nabla} - \frac{e}{c}\overrightarrow{A}\right)^2 - \left(\frac{V_0 e^{-2\delta r}}{1 - e^{-2\delta r}} - \frac{V_0' e^{-\delta r}}{r}\right)\right]\psi(r, \varphi) = E_{nm}\psi(r, \varphi), \tag{2.24}$$

where E_{nm} denotes the energy level, μ is the effective mass of the system, the vector potential which is denoted by "$\overrightarrow{A}$" can be written as a superposition of two terms $\overrightarrow{A} = \overrightarrow{A}_1 + \overrightarrow{A}_2$ having the azimuthal components [19] and external magnetic field with $\overrightarrow{\nabla} \times \overrightarrow{A}_1 = \overrightarrow{B}, \overrightarrow{\nabla} \times \overrightarrow{A}_2 = 0$, where $\overrightarrow{B}$ is the magnetic field. $\overrightarrow{A}_1 = \frac{\overrightarrow{B} e^{-\delta r}}{(1 - e^{-\delta r})}\widehat{\varphi}$ and $\overrightarrow{A}_2 = \frac{\varphi_{AB}}{2\pi r}\widehat{\varphi}$ represents the additional magnetic flux φ_{AB} created by a solenoid with $\overrightarrow{\nabla}.\overrightarrow{A}_2 = 0$ [19].

The vector potential in full is written in a simple form as [19];

$$\overrightarrow{A} = \left(0, \frac{\overrightarrow{B} e^{-\delta r}}{(1 - e^{-\delta r})} + \frac{\varphi_{AB}}{2\pi r}, 0\right) \tag{2.25}$$

From Eq. (2.24) we arrive at the following radial second-order differential equation:

$$R_{nm}''(r) + \frac{2\mu}{\hbar^2}\left[E_{nm} - V_{eff}(r)\right]R_{nm}(r) = 0 \tag{2.26}$$

$$V_{eff}(r) = -\frac{V_0 e^{-2\delta r}}{1 - e^{-2\delta r}} - \frac{V_0' e^{-\delta r}}{r} + \hbar\omega_c(m+\xi)\frac{e^{-\delta r}}{(1 - e^{-\delta r})r} + \left(\frac{\mu\omega_c^2}{2}\right)\frac{e^{-2\delta r}}{(1 - e^{-\delta r})^2}$$
$$+ \frac{\hbar^2}{2\mu}\left[\frac{(m+\xi)^2 - \frac{1}{4}}{r^2}\right] \tag{2.27}$$

where $\xi = \frac{\varphi_{AB}}{\varphi_0}$ is an integer with the flux quantum $\varphi_0 = \frac{hc}{e}$ and $\omega_c = \frac{e\overrightarrow{B}}{\mu c}$ denotes the cyclotron frequency.

Eq. (2.26) is not exactly solvable due to the presence of centrifugal term. Therefore, we employ the Greene and Aldrich approximation scheme [43,46] to overcome the centrifugal term. This approximation is given;

$$\frac{1}{r^2} \approx \frac{\delta^2}{(1 - e^{-\delta r})^2} \tag{2.28}$$

We point out here that this approximation is only valid for small values of the screening parameter δ. If we consider the approximation above, the effective potential of Eq. (2.27) is rewritten as follows:

$$V_{eff}(r) = P + Qz + Rz^2 \tag{2.29}$$

where we have introduced a new transformation given as $z = \frac{e^{-\delta r}}{1 - e^{-\delta r}}$. The dimensionless notations P, Q and R given below have been introduced also for simplicity:

$$P = \frac{\hbar^2\delta^2}{2\mu}\left((m+\xi)^2 - \frac{1}{4}\right), Q = \hbar\omega_c(m+\xi)\delta - V_0 - V_0'\delta + 2\left(\frac{\hbar^2\delta^2}{2\mu}\left((m+\xi)^2 - \frac{1}{4}\right)\right)$$
$$R = \frac{\hbar^2\delta^2}{2\mu}\left((m+\xi)^2 - \frac{1}{4}\right) + \hbar\omega_c(m+\xi)\delta + \frac{\mu\omega_c^2}{2} \tag{2.30}$$

Now, let us begin the application of the quantization rule to study the potential $V_{eff}(r)$. To perform this task, we have to first calculate the turning points z_a and z_b determined by solving $V(z) = E_{nm}$. Thus we have

$$z_a = -\frac{Q}{2R} - \frac{\sqrt{Q^2 - 4R(P - E_{nm})}}{2R} \tag{2.31}$$

$$z_b = -\frac{Q}{2R} + \frac{\sqrt{Q^2 - 4R(P - E_{nm})}}{2R} \tag{2.32}$$

with $k(z) = \sqrt{\frac{2\mu R}{\hbar^2}}\left[(z - z_a)(z - z_b)\right]^{\frac{1}{2}}$, \tag{2.33}

where $k(z)$ between the two turning points z_a and z_b.

Eq. (2.26) can also be written in the form of the Riccati equation as

$$-\delta z(1+z)\varphi_0'(z) + (\varphi_0(z))^2 + \frac{2\mu}{\hbar^2}\left[E_{nm} - P - Qz - Rz^2\right]\varphi_0(z) = 0 \qquad (2.34)$$

Considering the monotonic property, the logarithmic derivative form $\varphi_0(z)$ for the ground state has one node and no pole, thus we have to take a linear form in z. Therefore, we assume a trial solution of the form $\varphi_0(z) = A + Bz$, and substituting it into Eq. (2.34), we obtain the non-linear Riccati equation, we obtain the ground state energy as follows;

$$E_{0m} = P - \frac{\hbar^2 A^2}{2\mu} \qquad (2.35)$$

Also, A and B are as follows:

$$A = \frac{\delta}{2} + \frac{\mu Q}{\hbar^2 B} \text{ and } B = \frac{\delta}{2} \pm \sqrt{\frac{\delta^2}{4} + \frac{2\mu R}{\hbar^2}} \qquad (2.36)$$

while the problem can only be physically solvable for $B = \frac{\delta}{2} + \sqrt{\frac{\delta^2}{4} + \frac{2\mu R}{\hbar^2}}$. Let us now calculate the quantum correction. For this purpose, we utilised the integrals given by Appendix A, and we obtain

$$\int_{r_a}^{r_b} k_0'(r)\frac{\varphi_0}{\varphi_0}dr = -\int_{z_a}^{z_b}\frac{k_0'(z)}{\delta z(1+z)}\frac{\varphi_0(z)}{\varphi_0'(z)}dz = \frac{1}{\delta}\sqrt{\frac{2\mu R}{\hbar^2}}\int_{z_a}^{z_b}\frac{\left(z - \frac{(z_a+z_b)}{2}\right)\left(\frac{A}{B}+z\right)}{z(1+z)\sqrt{(z-z_a)(z-z_b)}}dz$$

$$\frac{1}{\delta}\sqrt{\frac{2\mu R}{\hbar^2}}\int_{z_a}^{z_b}\frac{dz}{\sqrt{(z-z_a)(z-z_b)}}\left(\frac{\left(\frac{A}{B}-1\right)\left(1+\frac{(z_a+z_b)}{2}\right)}{z+1} - \frac{\frac{A}{B}\left(\frac{z_a+z_b}{2}\right)}{z} + 1\right) \qquad (2.37)$$

The quantum correction term is therefore given as;

$$Q_c = \frac{\pi}{\delta}\sqrt{\frac{2\mu R}{\hbar^2}}\left[\frac{1}{B}\sqrt{\frac{2\mu R}{\hbar^2}} + 1\right] \qquad (2.38)$$

$$\int_{r_a}^{r_b} k(r)dr = -\int_{\sigma_a}^{\sigma_b}\frac{k(z)}{\delta z(1+z)}d\sigma$$
$$= -\frac{1}{\delta}\sqrt{\frac{2\mu R}{\hbar^2}}\int_{z_a}^{z_b}\frac{\sqrt{(z-z_a)(z-z_b)}}{z(1+z)}dz \qquad (2.39)$$
$$= -\frac{\pi}{\delta}\sqrt{\frac{2\mu R}{\hbar^2}}\left[\sqrt{(z_a+1)(z_b+1)} - 1 - \sqrt{z_a z_b}\right]$$
$$= -\frac{\pi}{\delta}\sqrt{\frac{2\mu R}{\hbar^2}}\left[\sqrt{\frac{R-Q+P-E_{nm}}{R}} - 1 - \sqrt{\frac{P-E_{nm}}{R}}\right]$$

where we used an appropriate standard integral in Appendix A. By combining the results obtained in Eqs. (2.37) and (2.38) i.e.

$$-\frac{\pi}{\delta}\sqrt{\frac{2\mu R}{\hbar^2}}\left[\sqrt{\frac{R-Q+P-E_{nm}}{R}} - 1 - \sqrt{\frac{P-E_{nm}}{R}}\right] = N\pi$$
$$+\frac{\pi}{\delta}\sqrt{\frac{2\mu R}{\hbar^2}}\left[\frac{1}{B}\sqrt{\frac{2\mu R}{\hbar^2}} + 1\right], \qquad (2.40)$$

By carrying out some simple algebraic manipulations, and using the expressions in Eq. (2.29), we obtain the energy of the Hulthen-Type potential plus Yukawa potential under influence of magnetic and AB fields with topological defects as follows;

$$E_{nm} = \frac{\hbar^2\delta^2}{2\mu}\left((m+\xi)^2 - \frac{1}{4}\right)$$
$$- \frac{\hbar^2}{8\mu}\left[\frac{\frac{2\mu V_0}{\hbar^2} + \frac{2\mu V_0'\delta}{\hbar^2} + \left(\frac{\mu\omega_c}{\hbar}\right)^2 - \delta^2\left((m+\xi)^2 - \frac{1}{4}\right) - (n\delta+B)^2}{(n\delta+B)}\right]^2 \qquad (2.41)$$

3. Thermodynamic properties of the Hulthen-type potential plus Yukawa potential

3.1. Partition function in the absence of external fields

To determine the thermodynamic properties such as entropy $S(\beta)$, Helmholtz free energy $F(\beta)$, internal energy $U(\beta)$, and specific heat capacity $C(\beta)$ for diatomic molecules considered in this work, we first calculate the partition function $Z(\beta)$ of the system [18,47]. The partition function of the selected diatomic molecules is written as

$$Z(\beta) = \sum_{n=0}^{n_{max}} e^{-\beta E_n} \qquad (3.1)$$

where $\beta = \frac{1}{k_B T}$, k_B, is the Boltzmann constant, T is the absolute temperature, $n = 0,1,2,... < n_{max}$, with n_{max} is the maximum quantum number given by.

Eq. (3.1) can be written as follows with $\beta = \frac{1}{k_B T}$ and with k_B is the Boltzmann constant. Now, in a bid to evaluate the partition function, the energy equation of eq. (19) is rewritten as follows;

$$E_{n\ell} = R\left(\frac{(n+P)^2 - Q}{(n+P)}\right)^2 \qquad (3.2)$$

where we have defined the following;

$$P = \frac{1}{2} + \sqrt{\frac{1}{4} + \ell(\ell+1)}, Q = \frac{\mu V_0}{2\hbar^2\delta^2} + \frac{\mu V_0'}{\hbar^2\delta} \text{ and } R = -\frac{\hbar^2\delta^2}{2\mu} \qquad (3.3)$$

for mathematical simplicity.

Hence, on substituting Eq. (3.2) into Eq. (3.1), we obtain;

$$Z(\beta) = \sum_{n=0}^{n_{max}} e^{-\beta R\left(\frac{(n+P)^2 - Q}{(n+P)}\right)^2} \qquad (3.4)$$

where

$$n_{max} = -P \pm \sqrt{Q} \qquad (3.5)$$

It should be noted that Eq. (3.5) represents the maximum quantum number. The summation in

$$Z(\beta) = \int_0^{n_{\max}} e^{-\beta R \left(\frac{(n+P)^2 - Q}{(n+P)} \right)^2} dn \qquad (3.6)$$

To evaluate the integral in Eq. (3.6), we carry out the process as follows;

$$Z(\beta) = \int_P^{n_{\max}+P} e^{-\beta R \left(\rho^2 + \frac{Q^2}{\rho^2} - 2Q \right)^2} d\rho \qquad (3.7)$$

where we have defined; $\rho = n + P$, and the integral is evaluated in the limits: $P \leq \rho \leq n_{\max} + P$.

The integral in Eq. (3.7) is now evaluated using Mathematica software to obtain partition function, $Z(\beta)$ as follows;

$$Z(\beta) = -\frac{e^{2QR\beta - 2\sqrt{R\beta}\sqrt{Q^2 R\beta}} \sqrt{\pi}}{4\sqrt{R\beta}} \left(\begin{array}{c} Erf\left[t_1 \sqrt{R\beta} - \frac{\sqrt{Q^2 R\beta}}{t_1} \right] + e^{4\sqrt{R\beta}\sqrt{Q^2 R\beta}} Erf\left[t_1 \sqrt{R\beta} + \frac{\sqrt{Q^2 R\beta}}{t_1} \right] \\ -Erf\left[t_2 \sqrt{R\beta} - \frac{\sqrt{Q^2 R\beta}}{t_2} \right] - e^{4\sqrt{R\beta}\sqrt{Q^2 R\beta}} Erf\left[t_2 \sqrt{R\beta} - \frac{\sqrt{Q^2 R\beta}}{t_2} \right] \end{array} \right) \qquad (3.8)$$

where $t_1 = P, t_2 = n_{\max} + P$ and *Erf* denotes the usual error function [18].

3.2. Partition function in the presence of external fields

Following the same procedure as above, we obtain the partition function in the presence of magnetic and Aharanov-Bohm fields as follows;

$$Z(\beta) = -\frac{e^{P_3\beta - 2\sqrt{-P_1\beta}\sqrt{-P_2^2 P_1\beta}} \sqrt{\pi}}{4\sqrt{P_1\beta}} \left(\begin{array}{c} Erf\left[x_1 \sqrt{-P_1\beta} - \frac{\sqrt{-P_2^2 P_1\beta}}{x_1} \right] + e^{4\sqrt{-P_1\beta}\sqrt{-P_2^2 P_1\beta}} Erf\left[x_1 \sqrt{-P_1\beta} + \frac{\sqrt{-P_2^2 P_1\beta}}{x_1} \right] \\ -Erf\left[x_2 \sqrt{-P_1\beta} - \frac{\sqrt{-P_2^2 P_1\beta}}{x_2} \right] - e^{4\sqrt{-P_1\beta}\sqrt{-P_2^2 P_1\beta}} Erf\left[x_2 \sqrt{-P_1\beta} - \frac{\sqrt{-P_2^2 P_1\beta}}{x_2} \right] \end{array} \right) \qquad (3.9)$$

where we have defined the following;

$$P_0 = \frac{\hbar^2 \delta^2}{2\mu} \left((m+\xi)^2 - \frac{1}{4} \right); P_1 = \frac{\hbar^2 \delta^2}{8\mu}; P_2 = \frac{2\mu V_0}{\hbar^2 \delta^2} + \frac{2\mu V_0'}{\hbar^2 \delta} + \left(\frac{\mu \omega_c}{\hbar \delta} \right)^2 - \left((m+\xi)^2 - \frac{1}{4} \right) x_1 = Q_0, x_2 = n_{\max} + Q_0; \ Q_0 = \frac{1}{2} + \sqrt{(m+\xi)^2 + \left(\frac{\mu \omega_c}{\hbar \delta} \right)^2 + \frac{2\mu \omega_c}{\hbar \delta}(m+\xi)} \qquad (3.10)$$

In what follows, all thermodynamic and magnetic properties of the Hulthen-Yukawa potential, such as the free energy, the entropy, total energy and the specific heat, can be obtained through the partition function of Eq. (3.9), $Z(\beta)$. These thermodynamic and magnetic functions for the diatomic molecules system can be calculated from the

following expressions [48-50];

$$F(\beta) = -\frac{1}{\beta} \ln Z(\beta),$$

$$U(\beta) = -\frac{d \ln Z(\beta)}{d\beta},$$

$$S(\beta) = \ln Z(\beta) - \beta \frac{d \ln Z(\beta)}{d\beta},$$

$$C(\beta) = \beta^2 \frac{d^2 \ln Z(\beta)}{d\beta^2}, \qquad (3.11)$$

$$M(\beta) = \frac{1}{\beta} \left(\frac{1}{Z(\beta)} \right) \left(\frac{\partial}{\partial \vec{B}} Z(\beta) \right),$$

$$\chi_m(\beta) = \frac{\partial M(\beta)}{\partial \vec{B}},$$

4. Results and discussion

In the present study, we use the energy spectrum to study the three selected diatomic molecules, *CrH*, *NiC* and *CuLi*. The spectroscopic parameters of these molecules are given in Table 1 and taken from Ref. [51]. We used the following conversions; $\hbar c = 1973.269 \ eV\overset{0}{A}$ and $1 \ amu = 931.5 \times 10^6 eV(\overset{0}{A})^{-1}$ for all computations [52].

In Fig. 1 (a & b), the energy spectra of the HYP for *CrH*, *NiC* and *CuLi*

diatomic molecules versus angular momentum quantum number and principal quantum number respectively. The energy of the system increases monotonically as n and ℓ increases respectively. In Fig. 2(a-e), we show a graphical representation of the thermal properties. We analyze how these properties vary with for different discrete values of $n_{\max}$ with *CrH*, *NiC* and *CuLi* diatomic molecules. Fig. 2(a) shows the partition function against $\beta = \frac{1}{kT}$ for various diatomic molecules. It can

Table 1

Spectroscopic constants of the diatomic molecules studied in the present work.

Molecules [51]	$\delta(\overset{o}{A}{}^{-1})$	$\mu(amu)$
CrH	1.52179	0.988976
NiC	2.25297	9.974265
CuLi	1.00818	6.259494

be seen that the partition function increases as the temperature increases. Fig. 2(b) shows the free energy against $\beta = \frac{1}{kT}$ for various diatomic molecules. It is seen that the free energy upsurges monotonically as the temperature increases. Fig. 2(c) shows the entropy against $\beta = \frac{1}{kT}$ for various diatomic molecules. It seen that the entropy declines as the temperature increases. Fig. 2(d) shows the mean energy against $\beta = \frac{1}{kT}$ for various diatomic molecules. It seen that the mean

energy declines as the temperature increases. Fig. 2(e) shows the specific heat capacity against $\beta = \frac{1}{kT}$ for various diatomic molecules. It can be seen that for the selected molecules studied, the specific heat capacity first peaks and then declines as the temperature increases.

In Fig. 3, the Plots of thermal properties of HYP against maximum quantum, n_{max} are shown at a fixed. Fig. 3(a) shows the plot of the partition function of HYP versus n_{max} for various diatomic molecules. The partition function increases with increasing n_{max}. Fig. 3(b) shows the plot of the free energy of HYP versus n_{max} for various diatomic molecules. It is seen that the free energy of the HYP model decreases with increasing n_{max}. Fig. 3(c) shows the entropy of HYP versus n_{max} for various diatomic molecules. The entropy of HYP increases monotonically as n_{max} increases. Fig. 3(d) shows the plot of the internal energy of HYP versus n_{max} for various diatomic molecules. The internal energy increases monotonically as n_{max} rises. Fig. 3(e) shows the specific heat
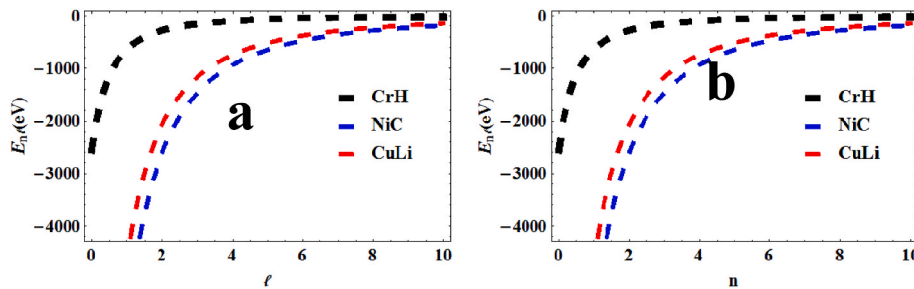

Fig. 1. Energy spectra of the HYP for CrH, NiC and $CuLi$ diatomic molecules versus: **(a)** Angular momentum quantum number **(b)** Principal quantum number.
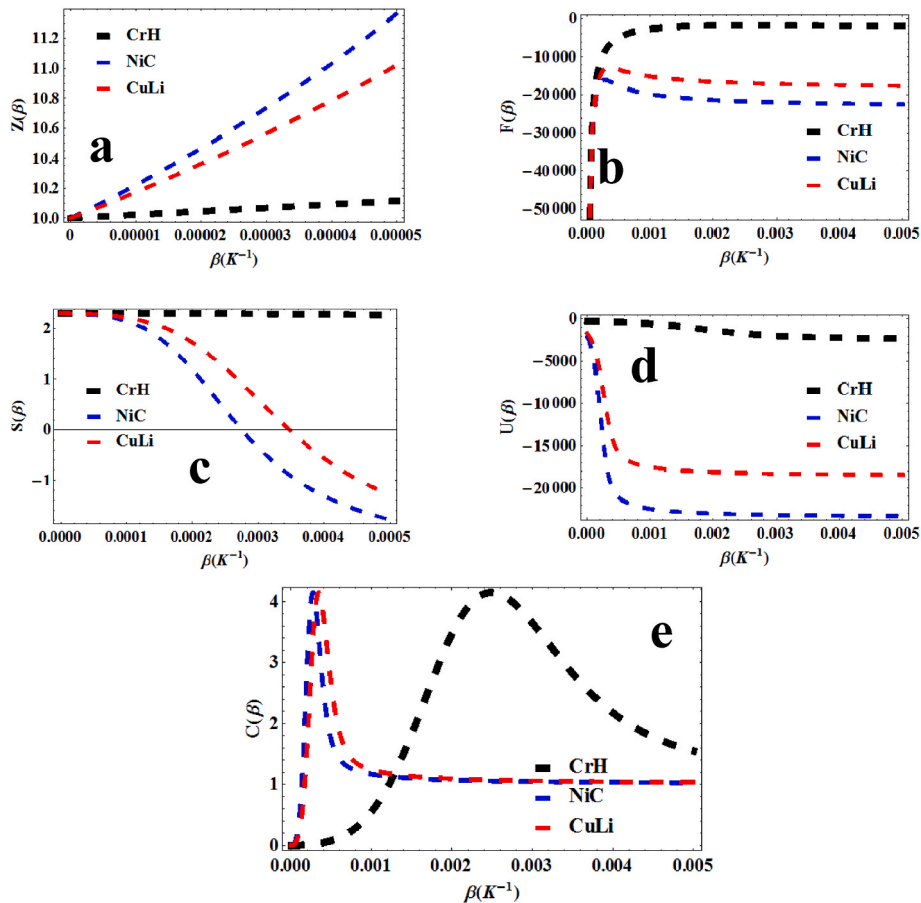

Fig. 2. Plots of thermal properties of HYP; (a) Partition function of HYP versus $\beta(K^{-1})$ for various diatomic molecules. (b) Free energy of HYP versus $\beta(K^{-1})$ for various diatomic molecules. (c) Entropy of HYP versus $\beta(K^{-1})$ for various diatomic molecules. (d) Internal energy of HYP versus $\beta(K^{-1})$ for various diatomic molecules. (e) specific heat capacity of HYP versus $\beta(K^{-1})$ for various diatomic molecules.
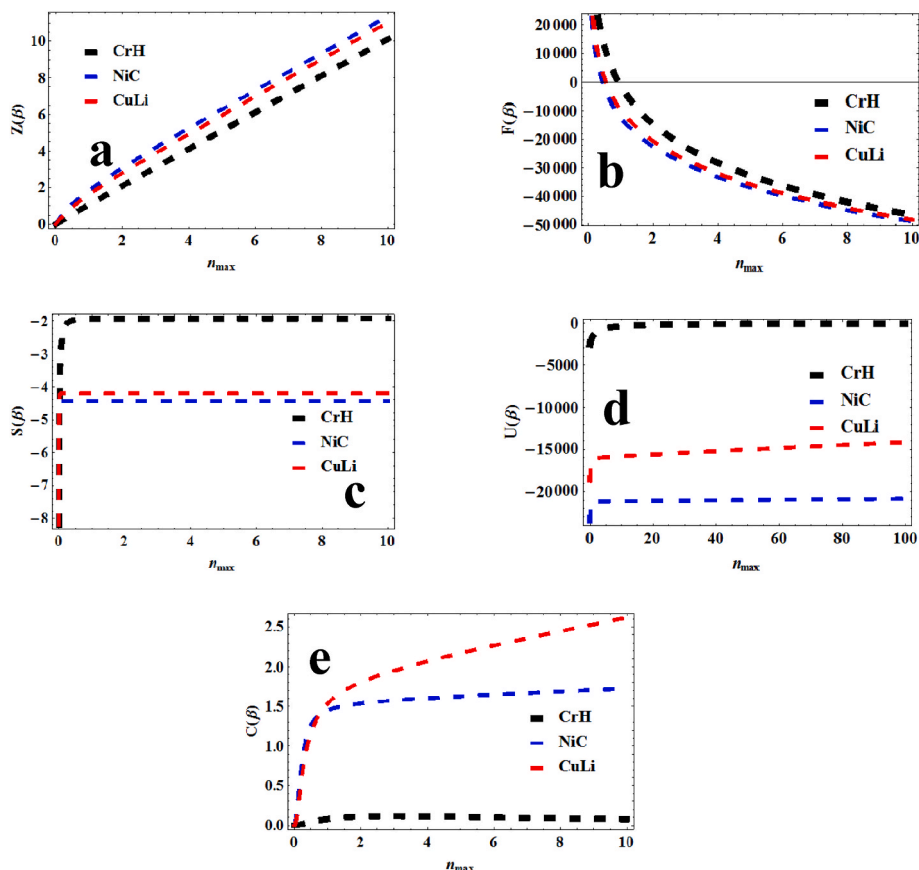
Fig. 3. Plots of thermal properties of HYP; (a) Partition function of HYP versus $n_{\max}$ for various diatomic molecules. (b) Free energy of HYP versus $n_{\max}$ for various diatomic molecules. (c) Entropy of HYP versus $n_{\max}$ for various diatomic molecules. (d) Internal energy of HYP versus $n_{\max}$ for various diatomic molecules. (e) specific heat capacity of HYP versus $n_{\max}$ for various diatomic molecules.

capacity of HYP versus $n_{\max}$ for various diatomic molecules. The specific heat capacity rises monotonically as $n_{\max}$ rises. Interestingly, we see that the specific heat capacity saturates at high $n_{\max}$. In addition, we note here that the specific heat capacity of *CrH* is seen to be quasi-invariant.

Fig. 4(a) shows the partition function against $\beta = \frac{1}{kT}$ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It can be seen that the partition function decreases as the temperature increases. Fig. 4(b) shows the free energy against $\beta = \frac{1}{kT}$ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It is seen that the free energy rises monotonically as the temperature increases. Fig. 4(c) shows the entropy against $\beta = \frac{1}{kT}$ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It seen that the entropy decays as the temperature upsurges. Fig. 4(d) shows the mean energy against $\beta = \frac{1}{kT}$ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It seen that the mean energy declines as the temperature increases. Fig. 4(e) shows the specific heat capacity against $\beta = \frac{1}{kT}$ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It can also be seen that for the selected diatomic molecules, the specific heat capacity decreases and attempts to rise for CrH.

Fig. 5(a) shows the partition function against $\vec{B}$ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It can be seen that the partition function decreases as the magnetic field increases. Fig. 5(b) shows the free energy against $\vec{B}$ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It is seen that the free energy rises as the magnetic field increases. Fig. 5(c) shows the entropy against $\vec{B}$ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It seen that the entropy

rises as the magnetic fields upsurges. Fig. 5(d) shows the mean energy against $\vec{B}$ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It seen that the mean energy increases as the magnetic fields increases. Fig. 5(e) shows the specific heat capacity against $\vec{B}$ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. Here, the specific heat capacity decreases and attempts to rise for CrH.

Fig. 6(a) shows the partition function against ξ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm (AB) fields. It can be seen that the partition function increases as the AB field increases. Fig. 6(b) shows the free energy against ξ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It is seen that the free energy decreases as the AB field increases. Fig. 6(c) shows the entropy against ξ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It seen that the entropy decreases as the AB fields upsurges but shows a quasi-linear or invariant trend for NiC and CuLi. Fig. 6(d) shows the mean energy against ξ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It seen that the mean energy decreases as the AB fields increases. Fig. 6(e) shows the specific heat capacity against ξ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It seen that for all molecules studied, the specific heat capacity does not shows a completely discernible trend in the variation pattern for NiC and CuLi and attempts to rise for CrH. Fig. 7(a) shows the magnetization against $\beta = \frac{1}{kT}$ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It can be seen that the magnetization increases as the temperature increases. Fig. 7(b) shows the magnetization against $\vec{B}$ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It is seen that the
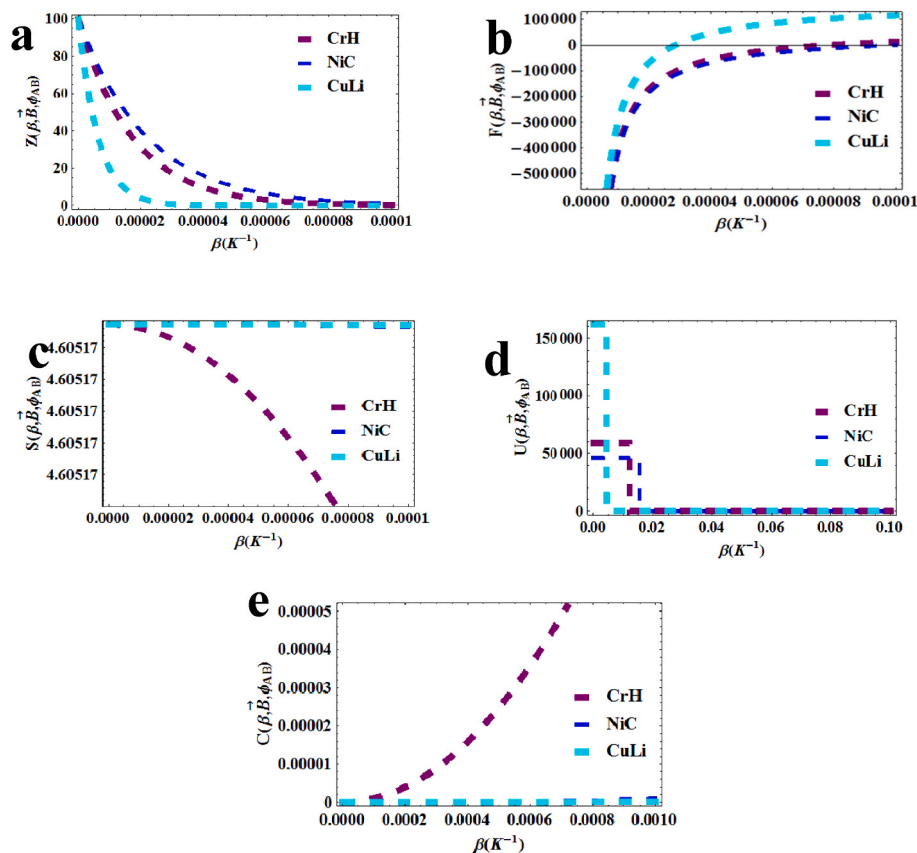
Fig. 4. Plots of thermal properties of HYP in the presence of magnetic and Aharanov-Bohm fields; (a) Partition function of HYP versus $\beta(K^{-1})$ for various diatomic molecules. (b) Free energy of HYP versus $\beta(K^{-1})$ for various diatomic molecules. (c) Entropy of HYP versus $\beta(K^{-1})$ for various diatomic molecules. (d) Internal energy of HYP versus $\beta(K^{-1})$ for various diatomic molecules. (e) specific heat capacity of HYP versus $\beta(K^{-1})$ for various diatomic molecules.

magnetization linearly decreases as the magnetic field increases. Fig. 7 (c) shows the magnetization against ξ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It seen that the magnetization does not vary as the AB field rises. Fig. 8(a) shows the magnetic susceptibility against $\beta = \frac{1}{kT}$ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It can be seen that the magnetic susceptibility rises as the temperature increases. Fig. 8(b) shows the magnetic susceptibility against $\overrightarrow{B}$ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It is seen that the magnetic susceptibility decreases as the magnetic field increases. Fig. 8(c) shows the magnetic susceptibility against ξ for various diatomic molecules in the presence of magnetic and Aharanov-Bohm fields. It seen that the magnetic susceptibility increases as the AB field rises.

5. Conclusion

In the present study, the focus is on solving the 3D Schrödinger equation has been solved with the Hulthen-Yukawa potential (HYP) within the framework of the Nikiforov-Uvarov method and 2D in the presence of magnetic and Aharanov-Bohm fields using exact quantization rule (EQR). The energy equation and the un-normalised wave function are acquired in both cases respectively. Furthermore, we study the thermodynamic properties of the HYP model for both cases. From the high temperature partition function obtained, thermodynamic functions, such as average energy $U(\beta)$, specific heat $C(\beta)$, free energy $F(\beta)$ and entropy $S(\beta)$ are gotten in the presence and absence of external magnetic and Aharanov-Bohm fields. It is found that in the classical limit, the specific heat capacity (in the absence of external perturbations) saturates for large values of the principal quantum number, n_{max} for the selected diatomic molecules at a fixed β except *CrH*. Also, we have plotted the variation of some of these thermodynamic functions as a function of β and n_{max}.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Appendix A. Nikiforov-Uvarov Method

The Nikiforov-Uvarov framework which through the coordinate system transforms the Schrödinger-like equations into hypergeometric-type second-order linear differential equation is given in the following form [53,54]
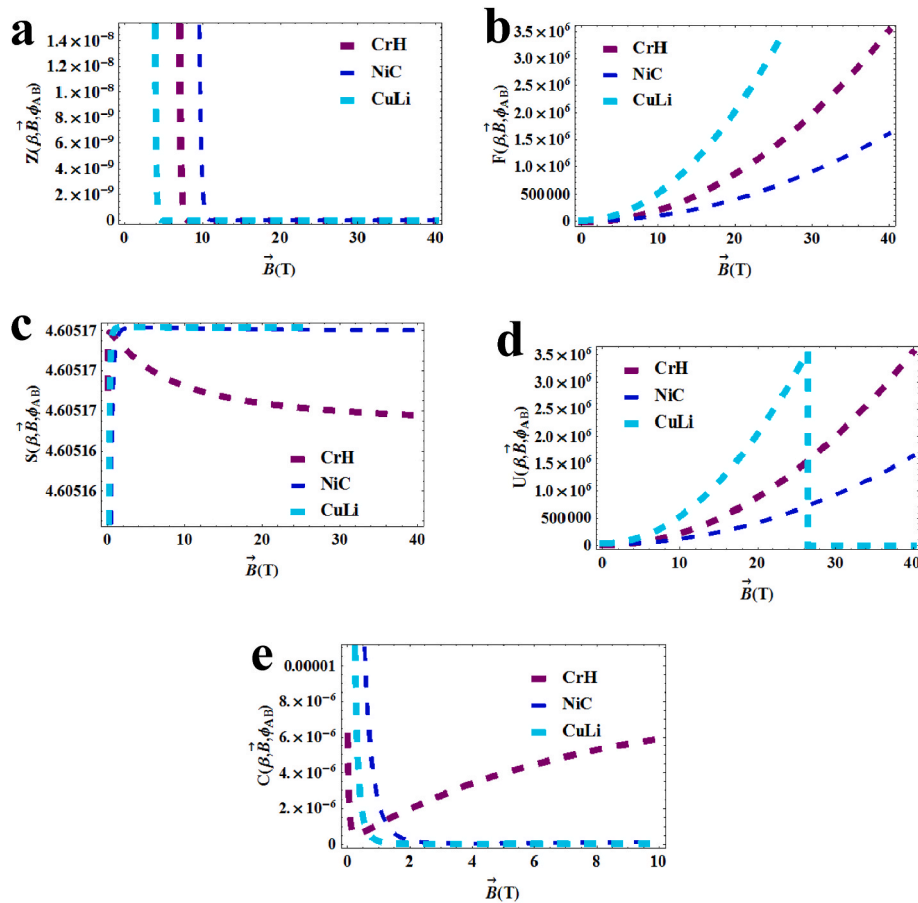
Fig. 5. Plots of thermal properties of HYP in the presence of magnetic and Aharanov-Bohm fields; (a) Partition function of HYP versus $\vec{B}$ for various diatomic molecules. (b) Free energy of HYP versus $\vec{B}$ for various diatomic molecules. (c) Entropy of HYP versus $\vec{B}$ for various diatomic molecules. (d) Internal energy of HYP versus $\vec{B}$ for various diatomic molecules. (e) specific heat capacity of HYP versus $\vec{B}$ for various diatomic molecules.

$$\psi''(s) + \frac{\widetilde{\tau}(s)}{\sigma(s)}\psi'(s) + \frac{\widetilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0 \qquad (A.1)$$

To obtain exact solution to eq. (A.1), we let the wave function be

$$\psi(s) = \varphi(s)y(s) \qquad (A.2)$$

By substituting eq. (92) into eq. (91), we obtain the hyper-geometric equation

$$\sigma(s)y_n''(s) + \tau(s)y_n'(s) + \lambda y_n(s) = 0 \qquad (A.3)$$

The wave function is given as

$$\frac{\varphi'(s)}{\varphi(s)} = \frac{\pi(s)}{\sigma(s)} \qquad (A.4)$$

For a fixed n, the hyper-geometric type function $y_n(s)$ is expressed in Rodrigues relation as

$$y_n(s) = \frac{B_n(s)}{\rho(s)} \frac{d^n}{ds^n}[\sigma^n(s)\rho(s)] \qquad (A.5)$$

Where B_n is the normalization constant and $\rho(s)$ the weight function which satisfies the condition below;

$$\frac{d}{ds}(\sigma(s)\rho(s)) = \tau(s)\rho(s) \qquad (A.6)$$

where also

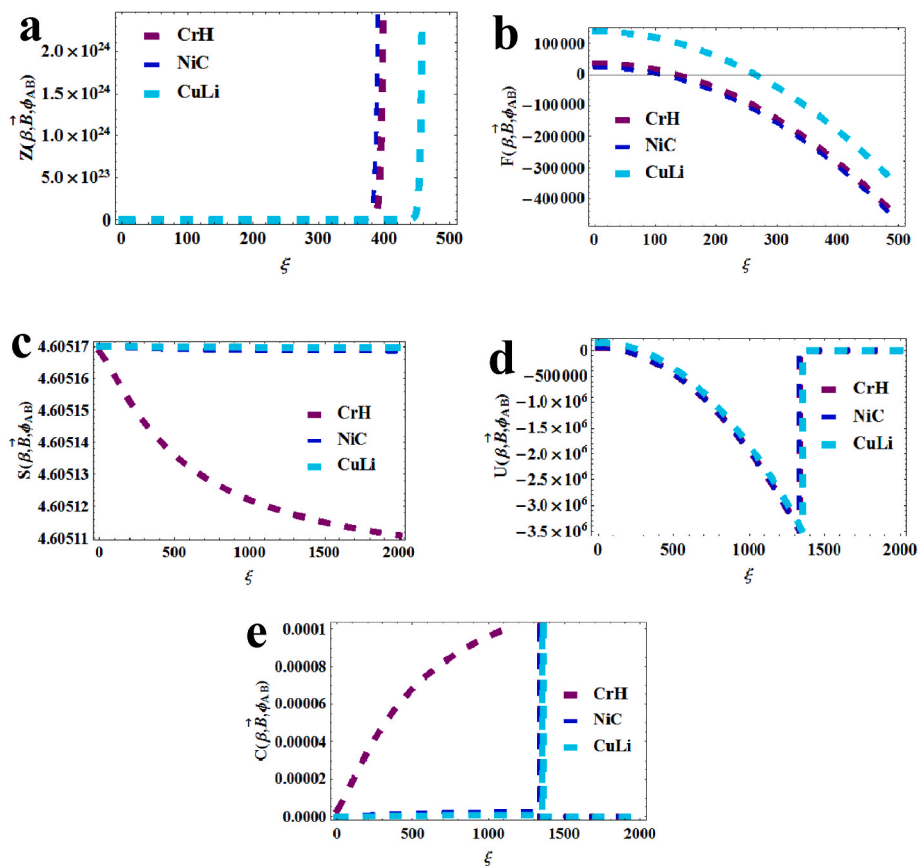$$\tau(s) = \widetilde{\tau}(s) + 2\pi(s) \qquad (A.7)$$

Fig. 6. Plots of thermal properties of HYP in the presence of magnetic and Aharanov-Bohm fields; (a) Partition function of HYP versus ξ for various diatomic molecules. (b) Free energy of HYP versus ξ for various diatomic molecules. (c) Entropy of HYP versus ξ for various diatomic molecules. (d) Internal energy of HYP versus ξ for various diatomic molecules. (e) specific heat capacity of HYP versus ξ for various diatomic molecules.
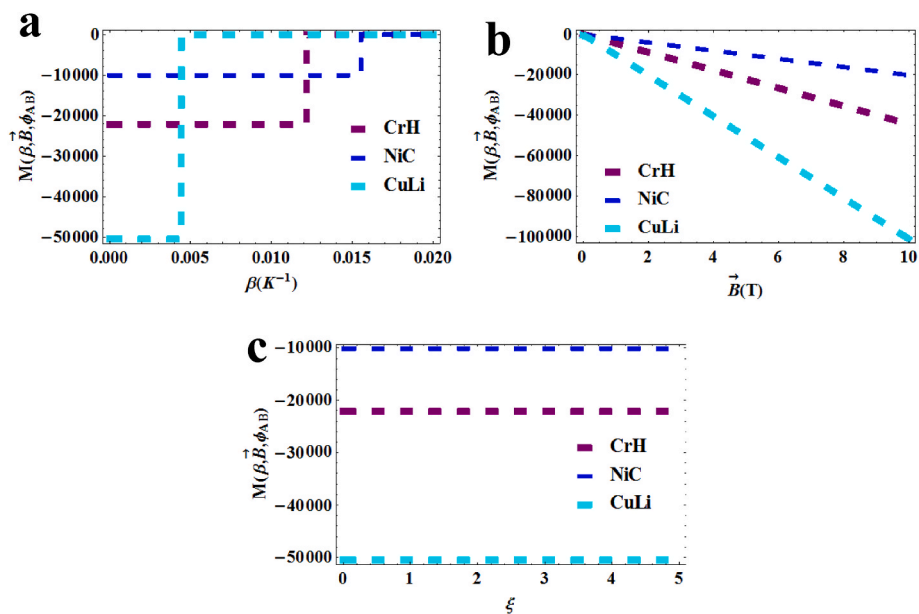

Fig. 7. Plots of magnetic properties of HYP in the presence of magnetic and Aharanov-Bohm fields; (a) Magnetization of HYP versus $\beta(K^{-1})$ for various diatomic molecules. (b) Magnetization of HYP versus $\vec{B}$ for various diatomic molecules. (c) Magnetization of HYP versus ξ for various diatomic molecules.
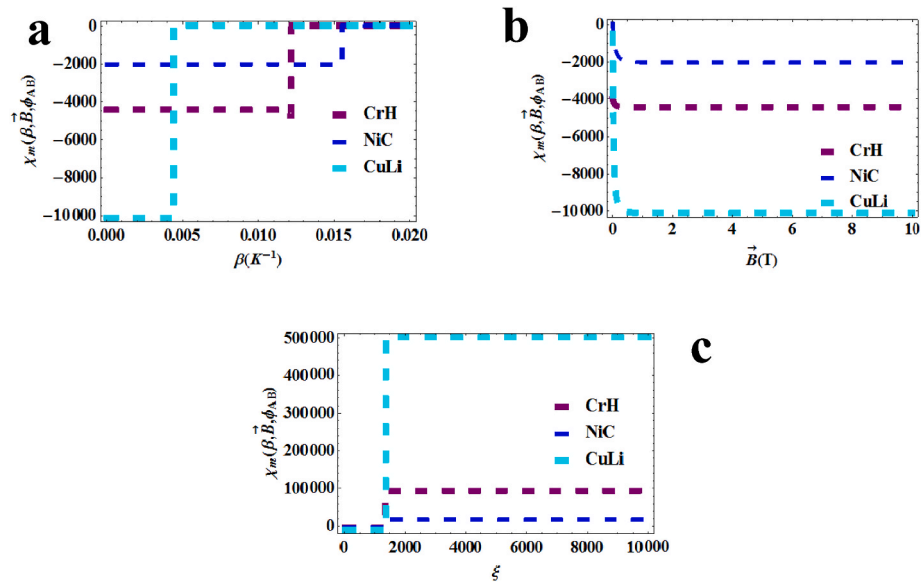
Fig. 8. Plots of magnetic properties of HYP in the presence of magnetic and Aharanov-Bohm fields; (a) Magnetic susceptibility of HYP versus $\beta(K^{-1})$ for various diatomic molecules. (b) Magnetic susceptibility of HYP versus $\vec{B}$ for various diatomic molecules. (c) Magnetic susceptibility of HYP versus ξ for various diatomic molecules.

For bound solutions, it is required that

$$\frac{d\tau(s)}{ds} < 0 \tag{A.8}$$

Therefore, the function $\pi(s)$ and the parameter λ required for the NU method are defined as

$$\pi(s) = \frac{\sigma'(s) - \widetilde{\tau}(s)}{2} \pm \sqrt{\left(\frac{\sigma'(s) - \widetilde{\tau}(s)}{2}\right)^2 - \widetilde{\sigma}(s) + k\sigma(s)} \tag{A.9}$$

$$\lambda = k + \pi'(s) \tag{A.10}$$

The values of k are obtained if the discriminant in the square root of eq. (A.9) vanish, so the new eigen equation becomes

$$\lambda_n = -\frac{nd\tau(s)}{ds} - \frac{n(n-1)}{2}\frac{d^2\sigma(s)}{ds^2} \tag{A.11}$$

$$n = 0, 1, 2, -$$

By equating eq. (A.10) and eq. (A.11), the energy eigenvalue is obtained.

Appendix B. Exact Quantization Rule (EQR)

A brief overview of the EQR is given in this section. A well detailed review can be found in Refs. [55-57]. It is established that, in one dimension, the SE is given as

$$\frac{d^2\psi(x)}{dx^2} + \frac{2\mu}{\hbar^2}[E - V(x)]\psi(x) = 0, \tag{B1}$$

can be re-written in the following form:

$$\varphi'(x) + \varphi(x)^2 + k(x)^2 = 0, \text{ with } k(x) = \sqrt{\frac{2\mu}{\hbar^2}[E - V(x)]}, \tag{B2}$$

where $\varphi(x) = \frac{\psi'(x)}{\psi(x)}$ is the logarithmic derivative of the wave function $\psi(x)$, the prime here denotes the derivative with respect to the variable x, μ denotes the reduced mass of the two interacting particles, $k(x)$ is the momentum, and $V(x)$ is a piecewise continuous real potential function of x. For the SE, the phase angle is the logarithmic derivative $\varphi(x)$. From (B2), as x increases across a node of wave function $\psi(x)$, $\varphi(x)$ decreases to $-\infty$, jumps to $+\infty$, and then decreases again.

Ma and Xu [55, 57] extended this exact quantization rule to the three-dimensional radial SE with spherically symmetric potential by simply making the replacements $x \rightarrow r$ and $V(x) \rightarrow V_{eff}(r)$:

$$\int_{r_a}^{r_b} k(r)dr = N\pi + \int_{r_a}^{r_b} \varphi(r)\left[\frac{dk(r)}{dr}\right]\left[\frac{d\varphi(r)}{dr}\right]^{-1}, \tag{B3}$$

with $k(r) = \sqrt{\frac{2\mu}{\hbar^2}[E - V_{eff}(r)]}$, where r_a and r_b are two turning points determined by $E_{n\ell} = V_{eff}(r)$. $N = n + 1$ is the number of the nodes of $\varphi(r)$ in the region $E_{n\ell} = V_{eff}(r)$ and is larger by 1 than the n of the nodes of wave function $\psi(r)$. The first term $N\pi$ is the contribution from the nodes of the logarithmic derivative of the wave function, and the second one is called the quantum correction. It was found that, for all well-known exactly solvable quantum systems, this quantum correction is independent of the number of nodes of the wave function. This means that it is enough to consider the ground state in calculating the quantum correction, i.e.,

$$Q_c = \int_{r_a}^{r_b} k_0'(r) \frac{\varphi_0}{\varphi_0'} dr \tag{B4}$$

Appendix C. Some Useful integrals employed in this study

$$\int_{r_a}^{r_b} \frac{1}{\sqrt{(r - r_a)(r_b - r)}} = \pi. \tag{C1}$$

$$\int_{r_a}^{r_b} \frac{1}{(a + br)\sqrt{(r - r_a)(r_b - r)}} dr = \frac{\pi}{\sqrt{(a + br_b)(a + br_a)}}. \tag{C2}$$

$$\int_{r_a}^{r_b} \frac{1}{r} \sqrt{(r - r_a)(r_b - r)} dr = \frac{\pi}{2}(r_a + r_b) - \pi\sqrt{r_a r_b}. \tag{C3}$$

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