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Non-relativistic solutions of the modified Hylleraas potential in the presence of external magnetic and Aharonov-Bohm flux fields for heteronuclear diatomic molecules

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In this study, we solve the Schrödinger equation with the modified Hylleraas potential (MHP) using the Nikiforov-Uvarov method in the presence of external magnetic and Aharonov-Bohm (AB) flux fields. We determine non-relativistic energy eigenvalues for various vibrational and magnetic quantum numbers, and examine the energy spectra of the MHP with and without these external fields for heteronuclear diatomic molecules like Carbon monoxide (CO) and hydrogen chloride (HCl). We observe that the presence of these fields increases the energy spectrum and breaks degeneracy. These findings could enable precision molecular spectroscopy, quantum control in molecular devices, and energy storage technologies. Additionally, we discover that the AB flux field has a more significant impact on the energy spectrum compared to the magnetic field. We also analyze the system's thermodynamic properties, including the partition function, mean energy, specific heat capacity, free energy, and entropy, providing valuable insights into its behavior. Generally, this study lays a foundation for further investigation into various quantum chemistry topics, highlighting how external fields can significantly influence the properties and behavior of molecular systems.

Key words: Thermodynamic properties; Schrödinger equation; Modified Hylleraas potential; Nikiforov-Uvarov method; Aharonov-Bohm flux.
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1 Introduction

The Schrödinger equation indeed lies at the focal point of the non-relativistic quantum mechanics, providing a fundamental framework for understanding the behavior of quantum systems. It's fascinating how, once solved, it encapsulates so much about a system, offering insights into its energy levels and wavefunctions [1-3]. Various potential models have been devised to describe interactions within quantum systems [4-6], and the modified Hylleraas potential model is one such approach. It is particularly useful in contexts where two charged particles interact, such as the nuclei in a diatomic molecule. The modified Hylleraas potential is valuable for understanding molecular structure and dynamics, offering unique advantages by accurately modeling both short- and long-range interactions. Unlike other potentials, it captures complex quantum behaviors and allows precise exploration of field-induced effects on molecular energy spectra, providing deeper insights into molecular dynamics and enhancing quantum chemistry applications.The diverse methods researchers have developed to solve the Schrödinger equation with these potential models demonstrate the depth of exploration in quantum mechanics and the ongoing quest to understand complex systems at the quantum level [7-11]. The modified Hylleraas potential is given as;

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

where V_o is the depth of the potential well, a and b are the potential parameters, α is the screening parameter. The modified Hylleraas potential (MHP)

model is a short-range potential that can be used to describe interactions within molecular, atomic, or nuclear systems [12]. The MHP has been used extensively in recent studies involving diatomic molecules [13,14]. Currently, the effect of *magnetic* and Aharanov-Bohm (AB) flux fields on energy spectrum of quantum systems have been on the forefront research [15,16]. For instance, the investigation by Edet [17] on the Yukawa potential energy spectra and the work by Horchani et al. [18] on the inversely quadratic Yukawa potential highlight the importance of understanding how external fields affect these systems. Additionally, Ikot et al. [19] contribute by emphasizing the significance of external fields on energy spectra and magnetic properties. The appealing effects of magnetic and AB field on the energy spectra, thermodynamics and magnetic properties of systems motivates us to study the impact of these fields on the modified Hylleraas potential. The motivation comes from the fact that this potential model fines very useful application in a wide area of specialties in physics and chemical physics. In this paper, we present the solution to the Schrodinger equation (SE) for the MHP model in the presence of magnetic and AB flux fields using the Nikifarov-Uvarov method. Then the energy obtained is applied to measure the partition function and other thermodynamic functions such as; entropy, mean energy, free energy, and specific heat capacity. This paper is structured as follows: In Section 2, we provide the solution to the Schrodinger equation for the modified Hylleraas potential, accounting for magnetic and AB fields. In Section 3, the thermodynamic properties of the potential model under consideration are evaluated. The discussion of our findings is presented in Section 4, and our conclusion is presented in Section 5.

2 Theoretical frameworks

The Schrodinger equation for a particle moving in a cylindrical coordinate system within the modified Hylleraas potential under the combined effect of magnetic and AB fields can be stated as;

$$\left[\frac{1}{2\mu}\left(i\hbar\vec{\nabla}-\frac{e}{c}\vec{A}\right)^2+\frac{V_o}{b}\frac{\left(a-e^{-2\alpha r}\right)}{\left(1-e^{-2\alpha r}\right)}\right]\psi(r,\varphi)=E_{mn}\psi(r,\varphi) \tag{2}$$

where E_{mn} is the energy eigenvalues, r is inter nuclear distance and μ is the reduced mass of the system. $\vec{A}$ is the vector potential written as a superposition of two terms $\vec{A}=\vec{A}_1+\vec{A}_2$ [16] having azimuthal component and external magnetic field with $\vec{\nabla}\times\vec{A}_1=\vec{B};\vec{\nabla}\times\vec{A}_2=0$, where $\vec{A}_1=\frac{1}{2}\left(\vec{B}\times\vec{r}\right)=\frac{\vec{B}r}{2}\hat{\varphi}$, $\vec{B}$ is the magnetic field perpendicular to the plane of transversal motion of the particle, and $\vec{A}_2=\frac{\phi_{AB}}{2\pi r}\hat{\varphi}$, ϕ_{AB} is the addition AB field created by a solenoid in a cylindrical coordinate [20].

The vector potential can be written more explicitly as;

$$\vec{A}=\left(\frac{\vec{B}r}{2}+\frac{\phi_{AB}}{2\pi r}\right)\hat{\varphi} \tag{3}$$

We define the wave function in Eq. (2) as $\psi(r,\varphi)=\frac{R(r)}{\sqrt{2\pi r}}e^{-im\varphi}$ where m is the magnetic quantum number and R(r) is the radial part of the wave function. Substituting the wave function and Eq. (3) into Eq. (2), we obtain a second order differential equation given as;

$$\frac{d^2R(r)}{d^2r}+\Im\frac{R(r)}{r^2}+\left(\frac{2\mu E}{\hbar^2}-\frac{\pi mB}{\phi_o}-\frac{\pi^2B^2r^2}{\phi_o^2}-\frac{2\pi\zeta B}{\phi_o}-\frac{2\mu V_o(a-e^{-2\alpha r})}{\hbar^2 b(1-e^{-2\alpha r})}\right)R(r)=0 \tag{4}$$

where $\Im = \frac{1}{4} - m^2 - m\zeta - \zeta^2$, $\phi_o = \frac{hc}{e}$ and $\zeta = \frac{\phi_{AB}}{\phi_o}$

The exact solution of Eq. (4) cannot be obtained; hence we find the approximate solution by introducing the Greene and Aldrich approximation [21] stated by Eq. (5) to handle the centrifugal term,

$$\frac{1}{r^2} = \frac{\alpha^2}{\left(1 - e^{-2\alpha r}\right)^2} \tag{5}$$

The approximation here is valid for very small values of the screening parameter α. The Greene and Aldrich approximation simplifies the centrifugal term by replacing the angular momentum term with an effective potential, making the problem analytically solvable. However, this approximation assumes that the centrifugal force is weak, which may not hold in systems with high angular momentum or when the external fields significantly alter the molecular dynamics. This limitation could lead to reduced accuracy, especially for higher quantum numbers or stronger field strengths, where the centrifugal term plays a more prominent role.Considering the approximation stated in Eq. (5) and the transformation $z = e^{-2\alpha r}$, Eq. (4) is rewritten in terms of the new variable z as

$$\frac{d^2R(z)}{dz^2} + \frac{(1-z)}{z(1-z)}\frac{dR(z)}{dz} + \frac{1}{z^2(1-z)^2}\left[-\gamma_1 z^2 + \gamma_2 z - \gamma_3\right]R(z) = 0 \tag{6}$$

where

$$\gamma_1 = \frac{2\mu E}{4\alpha^2\hbar^2} - \frac{\pi m B}{4\alpha^2\phi_o} - \frac{\pi\zeta B}{2\alpha^2\phi_o} - \frac{\mu V_o}{2\alpha^2\hbar^2 b}$$

$$\gamma_2 = -2\frac{2\mu E}{4\alpha^2\hbar^2} + 2\frac{\pi m B}{4\alpha^2\phi_o} + 2\frac{\pi\zeta B}{2\alpha^2\phi_o} + a\frac{\mu V_o}{2\alpha^2\hbar^2 b} + \frac{\mu V_o}{2\alpha^2\hbar^2 b}$$

$$\gamma_3 = \frac{2\mu E}{4\alpha^2\hbar^2} + \frac{\Im}{4} - a\frac{\mu V_o}{2\alpha^2\hbar^2 b} - \frac{\pi m B}{4\alpha^2\phi_o} - \frac{\pi^2 B^2}{4\phi_o^2} - \frac{\pi\zeta B}{2\alpha^2\phi_o}$$

Equation (6) is a hypergeometric type second order differential equation which solvable by the Nikiforov-Uvarov (NU) method. Comparing the Eq. (6) to the standard NU equation [22] stated by Eq. (7), we obtain the requisite polynomials given by (8).

$$\psi''(z) + \frac{\tilde{\tau}(z)}{\sigma(z)}\psi'(z) + \frac{\tilde{\sigma}(z)}{\sigma^2(z)}\psi(z) = 0 \tag{7}$$

$$\left.\begin{aligned} \tilde{\tau}(z) &= 1 - z \\ \sigma(z) &= z(1-z) \\ \sigma^2(z) &= z^2(1-z)^2 \\ \tilde{\sigma} &= \gamma_1 z^2 + \gamma_2 z + \gamma_3 \end{aligned}\right\} \tag{8}$$

Using the polynomials in Eq. (8), another useful polynomial $\pi(z)$ is obtained as prescribed by the NU method. A brief review of the NU method is as presented by [22]. The Nikiforov-Uvarov method is chosen for its efficiency in providing better analytical solutions to second-order differential equations, simplifying complex potential models like the modified Hylleraas potential under external fields.

$$\pi(z) = -\frac{Z}{2} \pm \sqrt{(\beta - k)Z^2 + (\gamma_2 + k)Z + \gamma_3} \tag{9}$$

where $\beta = \frac{1}{4} + \gamma_1$

Equating the discriminant of the quadratic expression within the square root sign to zero, and solving the ensuring equation for k.

$$k = -(\gamma_2 + 2\gamma_3) \pm 2\sqrt{\gamma_3}\sqrt{\beta + \gamma_2 + \gamma_3} \tag{10}$$

Accepting the negative solution of k and substituting it into Eq.(9), we have

$$\pi(z) = -\frac{z}{2} \pm \pm\left(\sqrt{\gamma_3} + \sqrt{\beta + \gamma_2 + \gamma_3}\right)z - \sqrt{\gamma_3} \quad (11)$$

We apply the relationship

$$\tau(z) = \bar{\tau}(z) + 2\pi(z) \quad (12)$$

Using Eqs. (8) and (11) another useful polynomial is obtained;

$$\tau(z) = 1 - 2z - -2\left(\sqrt{\gamma_3} + \sqrt{\beta + \gamma_2 + \gamma_3}\right)z - 2\sqrt{\gamma_3} \quad (13)$$

Taking the first derivative of $\tau(z)$, we have;

$$\tau'(z) = -2 - 2\sqrt{\gamma_3} - 2\sqrt{\beta + \gamma_2 + \gamma_3} \quad (14)$$

Equating the parameter λ defined by Eqs. (15) and (16) respectively, we obtain a quantity which contain the energy eigenvalues as given by Eq. (17)

$$\lambda_n = -n\tau'(z) + \frac{n(n-1)}{2}\sigma''(z) = 0 \quad (15)$$

$$\lambda = k_{-} + \pi'_{-}(z) \quad (16)$$

$$\gamma_3 = \left[\frac{-\frac{1}{2}\left[\left(n + \frac{1}{2} + \sqrt{\chi}\right)^2 + \frac{1}{4} + \rho\right]}{\left(n + \frac{1}{2} + \sqrt{\chi}\right)}\right]^2 \quad (17)$$

where $\chi = \beta + \gamma_2 + \gamma_3$
$\rho = \gamma_3 - \beta$

Substituting the parameters γ_1, γ_2 and γ_3 as earlier defined into Eq. (17), we obtain the non-relativistic energy eigenvalue of the MHP;

$$E_{nm} = \left[aV_o + \frac{\hbar\omega_c}{4}(m + \zeta) + \frac{\alpha^2\mu\omega_c^2}{8} - \frac{1}{4}\left(\frac{1}{4} - m^2 - m\zeta - \zeta^2\right) - \frac{1}{4}\left\{ \left(n + \frac{1}{2} + \sqrt{\chi}\right)^2 + \frac{\pi^2B^2}{4\phi_o^2} + \frac{a\mu V_o}{2\alpha^2\hbar^2 b} - \frac{\mu V_o}{2\alpha^2\hbar^2 b} \Big/ \left(n + \frac{1}{2} + \sqrt{\chi}\right) \right\} \right] \quad (18)$$

where $\chi = \frac{1}{4} + \frac{\pi^2B^2}{4\phi_o^2} - \frac{1}{4}\left(\frac{1}{4} - m^2 - m\zeta - \zeta^2\right)$,

$\omega_c = \frac{eB}{hc}$ is the cyclotron frequency and m is the magnetic quantum number given as $m = \ell + \frac{1}{2}$. For our purpose Eq. (18) can written in a more compact form as

$$E_{nm} = A_1 - \frac{\hbar^2\alpha^2}{2\mu}\left[\frac{(n + A_2)^2 + A_3}{n + A_2}\right]^2 \quad (19)$$

where

$$A_1 = aV_o + \frac{\hbar\omega_c}{4}(m + \zeta) + \frac{\alpha^2\mu\omega_c^2}{8} - \frac{1}{4}\left(\frac{1}{4} - m^2 - m\zeta - \zeta^2\right)$$

$$A_2 = \frac{1}{2} + \frac{1}{2}\sqrt{1 + \frac{\pi^2B^2}{\phi_o^2} - \left(\frac{1}{4} - m^2 - m\zeta - \zeta^2\right)}$$

$$A_3 = \frac{\pi^2B^2}{4\phi_o^2} + \frac{a\mu V_o}{2\alpha^2\hbar^2 b} - \frac{\mu V_o}{2\alpha^2\hbar^2 b}$$

3 Thermodynamic properties of the modifed Hylleraas potential

The thermodynamic properties of a system are easily obtained when the partition function of the system is known [23]. However, the partition function (PF) is determined by obtaining the summation of all possible vibration energy of the system. Given the energy spectrum of stated in Eq. (19), the partition function $Z(\beta)$ for the MHP at a finite temperature T, is calculated in terms of the Boltzmann factor.

$$Z(\beta)=\sum_{n=0}^{n_{max}} e^{(-\beta E_{mn})} \tag{20}$$

where $\beta=\frac{1}{k_B T}$, k_B is the Boltzmann constant.

By substituting the energy spectrum in Eq. (19) into Eq. (20), the partition function is given as

$$Z(\beta)= = \sum_{n=0}^{n_{max}} \text{Exp.}\left\{-\beta\left(A_1-\frac{\hbar^2\alpha^2}{2\mu}\left[\frac{(n+A_2)^2+A_3}{n+A_2}\right]^2\right)\right\} \tag{21}$$

$$\text{Let } x=\frac{\hbar^2\alpha^2}{2\mu}, q=-A_1, t=n+A_2, p=xA_3^2$$

The partition function $Z(\beta)$ becomes;

$$Z(\beta)=\sum_{n=0}^{n_{max}} \text{Exp}\left[\beta q+\beta x t^2-\frac{\beta p}{t^2}\right] \tag{22}$$

Writing Eq. (22) in integral form we have;

$$Z(\beta)=\int_0^{n_{max}} e^{xt^2\beta-\frac{p\beta}{t^2}+\beta q}dt \tag{23}$$

Using Maple 10.0 version, the partition function of Eq. (23) can be evaluated as

$$Z(\beta)=\frac{e^{xt\beta+\beta q\sqrt{-p\beta}}\left(\frac{2n_{max}e^{\frac{p\beta}{n_{max}^2}}}{\sqrt{-p\beta}}-2\sqrt{p}\sqrt{\beta}\sqrt{\pi}\,\frac{\text{erfi}\left(\frac{\sqrt{p}\sqrt{\beta}}{n_{max}}\right)}{\sqrt{-p\beta}}-2\sqrt{\pi}\right)}{2} \tag{24}$$

And the imaginary error function *erfi*(y) is defined as follows

$$erfi(y)=\frac{erf(iy)}{i}=\frac{2}{\sqrt{\pi}}\int_0^y e^{t^2}dt. \tag{25}$$

Using Eq. (24) other thermodynamic relations are found as follows:

(a) vibrational mean energy

$$U(\beta)=-\frac{\partial InZ(\beta)}{\partial\beta} \tag{26}$$

(b) Vibrational specific heat capacity

$$C(\beta)=k_B\beta^2\left(\frac{\partial^2 InZ(\beta)}{\partial^2\beta}\right) \tag{27}$$

(c) Vibrational free energy

$$F(\beta)=-k_B T InZ(\beta) \tag{28}$$

(d) Vibrational entropy

$$S(\beta)=k_B InZ(\beta)-k_B\beta\frac{\partial InZ(\beta)}{\partial\beta} \tag{29}$$

4 Results and discussion

The study of heteronuclear diatomic molecules such as carbon monoxide (CO) and hydrogen chloride (HCl) is crucial due to their diverse applications in atmospheric science, spectroscopy, and industrial processes. Their unique bond properties, dipole moments, and vibrational-rotational spectra provide critical insights into molecular dynamics, advancing chemical analysis, environmental monitoring, and quantum information systems. To validate our findings, we employed spectroscopic data from Table 1 to analyze the energy levels of HCl and CO under external magnetic and Aharonov-Bohm (AB) flux fields. The analysis utilized the following referenced values:

$$1 \text{ amu} = 931.494028 \text{ MeV}/c^2,$$
$$1\ cm^{-1} = 1.239841875\times10^{-4} eV, \text{ and}$$
$$\hbar c = 1973.29 \text{ eV A}$$

[24] in our calculations. Tables 2 and 3 present the energy levels for the modified Hylleraas potential of HCl and CO, respectively, considering the influence of AB flux field (ζ) and external magnetic field (B) across various magnetic (m) and vibrational (n) quantum numbers using Equation (19). The Aharonov-Bohm (AB) effect is a quantum mechanical phenomenon where a charged particle experiences a phase shift when moving around a region with a magnetic field, even if the magnetic field is zero along the particle's path. The AB flux field represents the effect of this phenomenon on the molecule's energy levels. We observed degeneracy when both fields are absent (ζ = B = 0) for m = 1 and m = -1. Under the exclusive influence of the magnetic field (B ≠ 0; ζ = 0), energy levels rise, eliminating degeneracy while retaining quasi-degeneracy. Sole exposure to the AB field (B = 0; ζ ≠ 0) abolishes degeneracy, confining the system further. Consequently, the combined impact of both fields surpasses individual effects, causing a significant shift in the system's energy spectrum. This suggests that the interaction between the AB flux field and the external magnetic field alters the energy levels in a more pronounced manner than either field acting alone. In Figures 1 to 5, we plotted the thermodynamic functions against the temperature for selected heteronuclear diatomic molecules. Figure 1 depicts the partition function for HCl and CO. It was observed that as the temperature increases the molecules energy decreases. This implies that at higher temperatures, the distribution of these molecules among their energy states decreases rather than increases. Also, Fig 2 indicates a shape increase in the mean energy at almost zero temperature and an exponential decrease as the temperature increases. This behavior is consistent with the Boltzmann distribution, which describes the distribution of energy among the different energy states of a system at thermal equilibrium. At higher temperatures, particles are distributed among a greater number of energy states, resulting in a decrease in the average energy per particle. In Fig. 3 we observed that there is a linear increase between the two molecules as both the specific heat capacity and temperature increases. The linear increase in specific heat capacity with temperature may be indicative of various physical processes occurring within the molecules as temperature rises. For example, in gases, increasing temperature leads to greater molecular motion and vibrational modes becoming active, which require more energy to excite. In solids, higher temperatures may lead to increased thermal expansion and more pronounced lattice vibrations, contributing to higher specific heat capacities. Fig. 4 shows a rapid increase in free energy at a constant temperature and it begins to converge when the temperature increases. The rapid increase in free energy at constant temperature may correspond to the onset of a phase transition or chemical reaction, where the system undergoes a significant change in its internal structure or composition. The convergence of free energy with increasing temperature may indicate the stabilization of the system as temperature increases, leading to a reduction in the rate of change of free energy with temperature. The entropy against temperature is plotted in Fig. 5. We observed that as the temperature increase, the molecules entropy is seen to increase. The observed increase in entropy with increasing temperature is consistent with the general trend observed in many systems. As the temperature rises, the molecules in the system gain more thermal energy, leading to increased molecular motion and a greater number of accessible microstates. This increased molecular disorder contributes to an overall increase in the system's entropy. The increase in entropy with temperature has significant implications for various physical and chemical processes. For example, in phase transitions such as melting or vaporization, the increase in entropy with temperature plays a crucial role in determining the conditions under which these transitions occur.

Table 1 – Spectroscopic parameters of the selected heteronuclear diatomic molecules [25].

Molecules	$D_e(eV)$	$\alpha^{-9}\left(\mathring{A}^{-1}\right)$	$r_e(\mathring{A})$	$\mu(MeV)$
HCl	4.6190309050	1.86770	1.2746	0.09129614886
CO	11.225600000	2.29940	1.1283	0.63906749030

Table 2 – Eigenvalues (eV) for the modified Hylleraas potential for CO molecule with and without *B* and *AB* flux fields.

m	**n**	B = 0; $\zeta = 0$	B = 5 T; $\zeta = 0$	B = 0; $\zeta = 5$	B = 5 T; $\zeta = 5$
1	0	-10:89413685	-10:89412694	-10:88701166	-10:88700163
	1	-10:79366351	-10:79365356	-10:78663755	-10:78662748
	2	-10:69458650	-10:69457650	-10:68765794	-10:68764782
	3	-10:59688007	-10:59687002	-10:59004712	-10:59003695
0	0	-10:89437452	-10:89436462	-10:88843594	-10:88842593
	1	-10:79389787	-10:79388793	-10:78804200	-10:78803194
	2	-10:69481761	-10:69480762	-10:68904293	-10:68903282
	3	-10:59710798	-10:59709795	-10:59141299	-10:59140284
-1	0	-10:89413685	-10:89412696	-10:88938567	-10:88937567
	1	-10:79366351	-10:79365358	-10:78897851	-10:78896846
	2	-10:69458650	-10:69457652	-10:68996645	-10:68995636
	3	-10:59688007	-10:59687004	-10:59232377	-10:59231363

Table 3 – Eigenvalues (eV) for the modified Hylleraas potential for HCl molecule with and without *B* and *AB* flux fields.

m	**n**	B = 0; $\zeta = 0$	B = 5 T; $\zeta = 0$	B = 0; $\zeta = 5$	B = 5 T; $\zeta = 5$
1	0	-3:962892968	-3:962876513	-3:911543641	-3:911526223
	1	-3:805044609	-3:805027813	-3:756800366	-3:756782607
	2	-3:656677388	-3:656660250	-3:611292839	-3:611274738
	3	-3:517046921	-3:517029442	-3:474300445	-3:474282003
0	0	-3:964628515	-3:964612149	-3:921703713	-3:921686402
	1	-3:806674860	-3:806658153	-3:766347643	-3:766329991
	2	-3:658210692	-3:658193643	-3:620275626	-3:620257633
	3	-3:518490814	-3:518473424	-3:482762382	-3:482744047
-1	0	-3:962892968	-3:962876683	-3:928507319	-3:928490109
	1	-3:805044609	-3:805027984	-3:772740459	-3:772722907
	2	-3:656677388	-3:656660421	-3:626290068	-3:626272175
	3	-3:517046921	-3:517029612	-3:488427730	-3:488409495

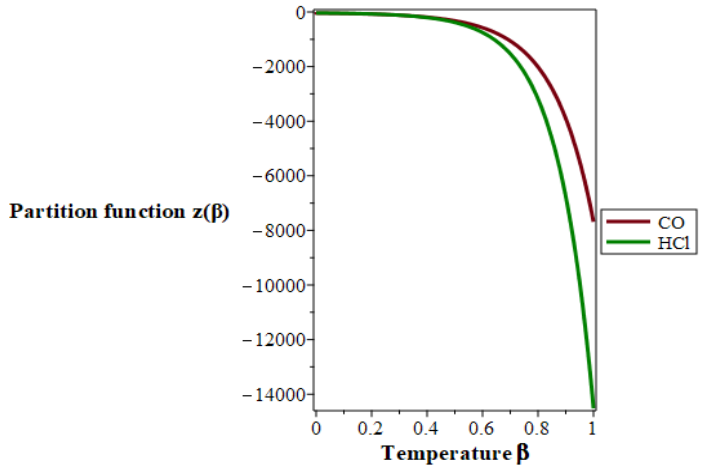

Figure 1 – Variation of the partition function $Z(\beta)$ versus temperature (β) for selected heteronuclear diatomic molecules.

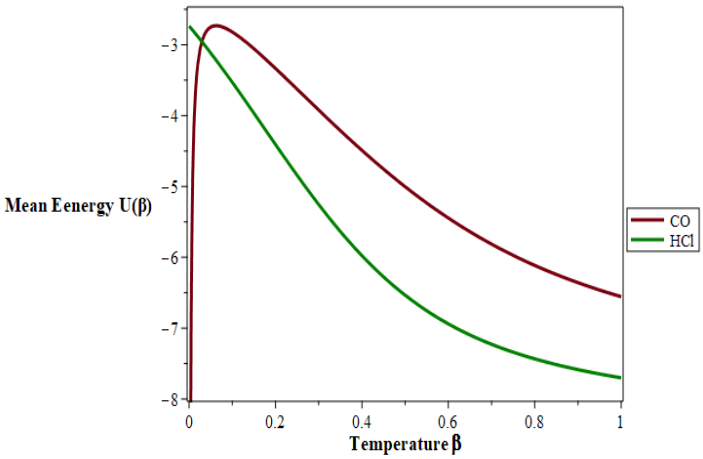

Figure 2 – Variation of the mean energy $U(\beta)$ versus temperature (β) for selected heteronuclear diatomic molecules.

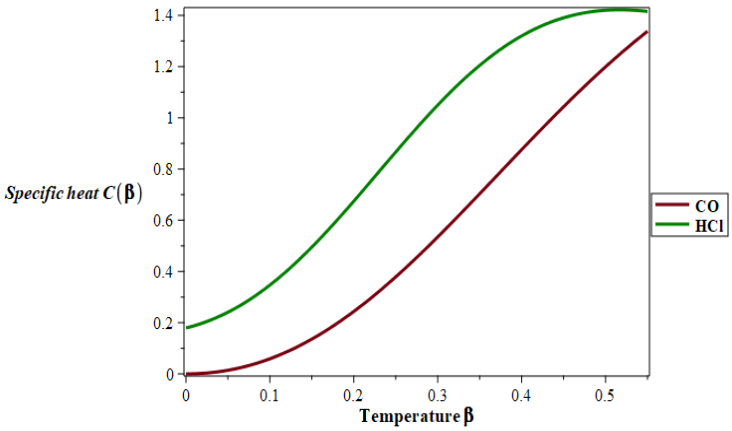

Figure 3 – Variation of the specific heat $C(\beta)$ versus temperature (β) for selected heteronuclear diatomic molecules.

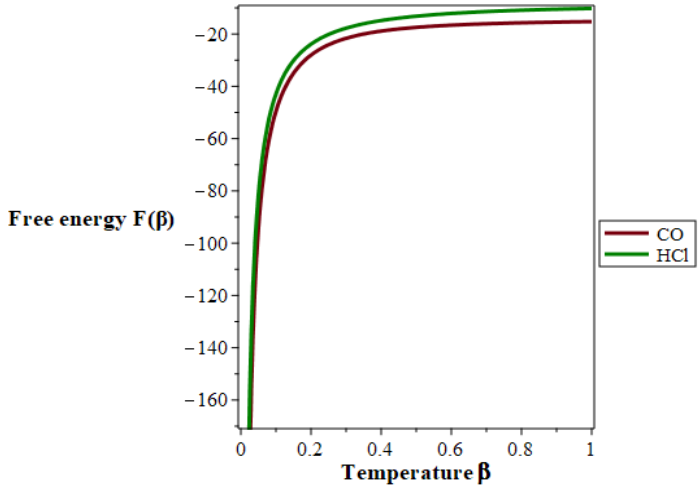

Figure 4 – Variation of the free energy $F(\beta)$ versus temperature (β) for selected heteronuclear diatomic molecules.

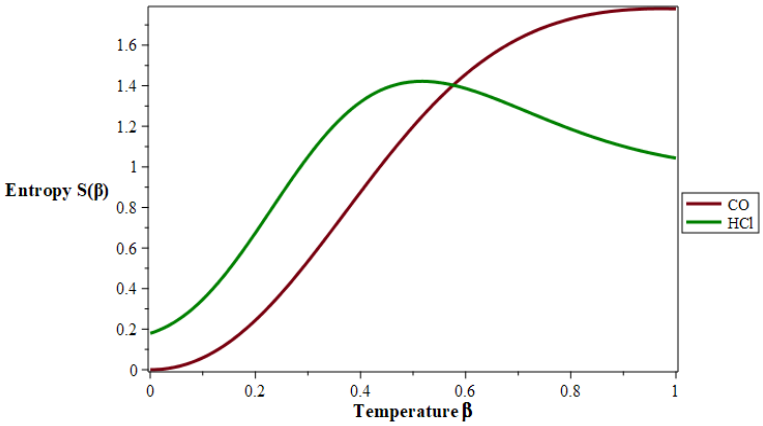

Figure 5 – Variation of the entropy $S(\beta)$ versus temperature (β) for selected heteronuclear diatomic molecules.

5 Conclusion

This work presents an analytical solution to the Schrödinger equation (SE) with the modified Hylleraas potential using the Nikiforov-Uvarov (NU) method, incorporating external magnetic and Aharonov-Bohm (AB) flux fields. The study calculates non-relativistic energy eigenvalues for various vibrational and magnetic quantum numbers and examines the influence of these fields on the energy spectra of heteronuclear diatomic molecules like CO and HCl. Degeneracy is observed in the absence of external fields, while the application of a magnetic field increases energy eigenvalues, breaking degeneracy but leaving some quasi-degeneracy. The AB field has a stronger effect, further reducing degeneracy and raising energy levels compared to the magnetic field. When both fields are applied, their combined impact exceeds their individual effects. The thermodynamic properties of the system, including the partition function, mean energy, specific heat capacity, free energy, and entropy, are analyzed and visualized, providing deeper insights into molecular behavior under external fields. This study establishes a foundation for exploring various quantum chemistry topics, illustrating how external fields can significantly influence molecular properties. The findings have implications for quantum technology development

and molecular physics, enabling advancements in field-tunable molecular systems for quantum sensors, quantum information processing, and advanced material design. Future research could extend these methods to more complex molecular systems and investigate the effects of diverse external field configurations.

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