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CONFORMABLE SCHRÖDINGER EQUATION WITH PSEUDOHARMONIC POTENTIAL AND ITS THERMODYNAMIC PROPERTIES

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In this work, the Nikiforov-Uvarov (NU) method is used to obtain the exact solution of the conformable radial Schrödinger equation (SE) for the pseudoharmonic potential. We derive both the energy states and the corresponding wave functions, and the results are compared with those in the existing literature for the case of the traditional derivative ($\alpha = 1$). Additionally, the obtained energy states are used to calculate the conformable partition function in the classical limit. Thermodynamic properties, including the conformable Helmholtz free energy, conformable mean energy, conformable entropy, and conformable specific heat capacity, are calculated and analyzed for N_2 and CO molecules.

Keywords: *Nikiforov-Uvarov method; Pseudoharmonic potential; Thermodynamic properties; Conformable partition function*

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1. INTRODUCTION

The exact solution of the Schrödinger wave equation for various potentials has been an attractive area of research for scientists in theoretical physics and related fields over the past several decades [1, 2, 3, 4, 5]. These solutions are important in both relativistic and non-relativistic regimes due to their significant role in statistical physics, solid-state physics, quantum field theory, and molecular physics. Such solutions provide complete information about quantum systems, including thermodynamic properties, mass spectra, and optical characteristics [6, 7, 8]. Several methods for solving Schrödinger wave equations have been reported to date, among which are the Nikiforov-Uvarov method [9, 10, 11], the factorization method [12, 13, 14], the series expansion method [15], and the functional analysis approach [16]. Among them, the NU method, originally developed to solve second-order differential equations of the hypergeometric type, has been widely applied to time-independent quantum problems [17].

Many scientists, including Riemann-Liouville, Caputo, and Riesz, have made significant contributions to the development of definitions for non-integer derivatives and their applications in physics [19, 20, 21, 22].These definitions take various forms, but most of them include operators of fractional derivatives that act as non-local operators. Thus, many of the basic properties of integer derivatives, such as the product and chain rules, do not hold for fractional derivatives. This makes algebraic operations in non-integer calculus challenging, as these foundational principles cannot be directly applied. To address these challenges, a new definition, known as the conformable fractional derivative, has been introduced [18].This definition provides many classical properties of derivatives and is thus more applicable in practical applications; the formal definition of such a derivative is given below in Equation 1.

$$D^{\alpha}[f(x)] = \lim_{\varepsilon\to 0}\frac{(f(x+\varepsilon x^{1-\alpha}) - f(x))}{\varepsilon}, x > 0 \tag{1}$$

where $0 < \alpha \leq 1$, this definition reduces to the classical definition of the first derivative when $\alpha = 1$. More properties of the conformable fractional derivative can be found in [18]. A significant number of studies have been conducted in recent years to extend the definition and express mathematical tools using conformable derivative notation, making it ready for use in applied sciences [23, 24, 25, 26]. In quantum physics, the conformable fractional NU method has been developed and applied to investigate solutions of the conformable SE for various potentials [27, 35]. Conformable mechanics could introduce new ways to engineer and interact with quantum systems, enhancing control, flexibility, and precision while potentially enabling new quantum phenomena and applications across quantum computing, sensing, and communication.

Many studies have explored the implications of the conformable derivative on classical and quantum mechanics. Reference [38] examines some applications of the conformable derivative in physics, including a detailed discussion of the divergence and Green's theorem. Additionally, the basics of Newtonian mechanics in the context of conformable derivatives are covered. While the conformable equation for hydrogen-like systems is discussed by Al-Masaeed et al [36], the analytical solutions are obtained for the angular part in terms of conformable Laguerre functions. Furthermore, the

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deformation of special relativity within the framework of conformable derivatives is formulated by Al-Jamel et al [39]. In this work, we will deal with the pseudoharmonic oscillator, which has the form [32]:

$$V(r) = D_e(\frac{r}{r_0} - \frac{r_0}{r})^2 \tag{2}$$

Where, D represents the dissociation energy between two atoms, and r_0 the equilibrium intermolecular separation. The pseudoharmonic oscillator is one of the most important molecular potentials in chemical physics, molecular physics, and related areas, due to its numerous applications in studying diatomic molecules. In fact, the significance of using pseudoharmonic potentials lies in their ability to more accurately describe real physical systems, especially in cases where the simple harmonic approximation breaks down. By incorporating anharmonic corrections, pseudoharmonic potentials provide a better fit for vibrational, thermodynamic, and molecular dynamics calculations, making them an essential tool in the study of complex systems in physics and chemistry. The pseudoharmonic potential is a useful tool for modeling anharmonicity in molecular and atomic systems, but it has limitations in its ability to capture strong anharmonicity, large displacements, or complex multi-body interactions. In cases where these limitations are important, more sophisticated potentials may be needed. The essential advantage of the SE with this potential consists in the fact that it allows one to get the exact solution for every rotational quantum number l [28, 29, 30, 37]. This is in contrast to the other molecular potentials, e.g., Morse potential that can be solved exactly for non-rotating diatomic molecules [31].

This work aims to solve the conformable SE for the pseudoharmonic potential using the Nikiforov-Uvarov method. The goal is to obtain the relevant energy spectrum and wave functions for a general conformable derivative of order α and to compare the findings with the existing literature for the specific case where $\alpha = 1$. Additionally, the present study also aims to derive the expression for the conformable partition function in the classical limit and calculate associated thermodynamic properties, such as the conformable vibrational mean energy, conformable specific heat, conformable free energy, and conformable entropy. Solving the conformable SE expands the applicability of quantum mechanical principles to more general and complex systems, supporting current research that aims to better understand and predict behaviors in diverse areas of physics and quantum computing.

2. CONFORMABLE SCHRÖDINGER EQUATION WITH PSEUDOHARMONIC POTENTIAL

The SE in three dimensions, when expressed in spherical coordinates (r, θ, ϕ) takes the form of a partial differential equation. In spherical coordinates, the time-independent SE for a particle with a potential $V(r, \theta, \phi)$ is given by:

$$\frac{-\hbar^2}{2m}\nabla^2\psi(r,\theta,\phi) + V(r,\theta,\phi)\psi(r,\theta,\phi) = E\psi(r,\theta,\phi) \tag{3}$$

To solve this equation, it is common to assume that the wavefunction can be separated into radial and angular components. In this work, we will focus on the conformable radial SE, as it varies for each system. However, the angular part has been solved in previous studies, as outlined in [36]. The radial SE is given by:

$$\frac{d^2R(r)}{dr^2} + \frac{2}{r}\frac{dR(r)}{dr} + \frac{2\mu}{\hbar^2}(E_{nl} - V(r) - \frac{l(l+1)\hbar^2}{2\mu r^2})R(r) = 0 \tag{4}$$

Where μ is the reduced mass, n and l denote the quantum numbers. Using relation (2) and the change of variable ($r = s^{\frac{1}{2}}$), the SE for the Pseudoharmonic potential takes the form [33]:

$$\frac{d^2R}{ds^2} + \frac{3/2}{s}\frac{dR}{ds} + \frac{1}{s^2}[-\gamma^2 s^2 - \epsilon s - \beta]R(s) \tag{5}$$

where

$$\gamma = \sqrt{\frac{D_e}{r_0}\frac{\mu}{2\hbar^2}} \qquad \epsilon = [E_{nl} + 2D_e]\frac{\mu}{2\hbar^2} \qquad \beta = (D_e r_0^2 + \frac{l(l+1)\hbar^2}{2\mu})\frac{\mu}{2\hbar^2} \tag{6}$$

Now, we would like to express the SE for Pseudoharmonic potential in terms of conformable derivative as follows:

$$D^\alpha D^\alpha R(s) + \frac{3/2}{s}D^\alpha R(s) + \frac{1}{s^2}[-\gamma^2 s^2 - \epsilon s - \beta]R(s) \tag{7}$$

Using the properties of conformable fractional derivative [18]

$$D^\alpha R(s) = s^{(1-\alpha)}R(s)$$

$$D^\alpha D^\alpha R(s) = (1-\alpha)s^{(1-2\alpha)}\frac{dR}{ds} + s^{(2-2\alpha)}\frac{d^2R}{ds^2}$$

The conformable SE for pseudoharmonic potential can be written as:

$$R''(s) + \frac{\frac{5}{2} - \alpha}{s}R'(s) + \frac{1}{s^2}[-\gamma^2 s^{2\alpha} - \epsilon s^\alpha - \beta]R(s) \tag{8}$$

Next, we compare the Conformable equation (8) with the basic equation of traditional NU method

$$\psi''(s) + \frac{\tilde{\tau_f}(s)}{\sigma_f(s)}\psi'(s) + \frac{\tilde{\sigma}}{\sigma_f^2}\psi(s) \tag{9}$$

The parameters in Eq (9) can be determined as:

$$\tilde{\tau_f}(s) = \frac{5}{2} - \alpha \qquad \tilde{\sigma_f}(s) = [-\gamma^2 s^{2\alpha} + \epsilon s^\alpha - \beta] \qquad \sigma_f(s) = s \tag{10}$$

The function $\pi_f(s)$ and parameter λ which are given by NU read as:

$$\pi_f(s) = \frac{D^\alpha(\sigma_f(s)) - \tilde{\tau}_f(s)}{2} \pm \sqrt{(\frac{D^\alpha(\sigma_f(s)) - -\tilde{\tau}_f(s)}{2})^2 - \tilde{\sigma_f}(s) + k\sigma_f(s)} \qquad \lambda(s) = K(s) + D^\alpha \pi_f(s) \tag{11}$$

Which can be calculated for our problem as:

$$\pi_f(s) = \frac{-3s^{\alpha-1}}{4} + \frac{\alpha}{2} \pm \sqrt{[\frac{-3s^{\alpha-1}}{4} + \frac{\alpha}{2}]^2 - [-\gamma^2 s^{2\alpha} + \epsilon s^\alpha - \beta] + ks^\alpha} \tag{12}$$

To solve the quadratic equation inside the square root in Eq (12), the discriminant must be set to zero. This condition leads to a new quadratic equation, which can then be solved to determine the constant $K(s)$, ensuring the existence of both roots.

$$K_1 = \epsilon + 2\gamma\sqrt{\frac{\alpha^2}{4} - \frac{12\alpha}{16} + \beta + \frac{9}{16}} \qquad K_2 = \epsilon - 2\gamma\sqrt{\frac{\alpha^2}{4} - \frac{12\alpha}{16} + \beta + \frac{9}{16}} \tag{13}$$

Substituting the two values of K from Eq (13) into Eq (12) yields four possible forms of $\pi_f(s)$:

$$\pi_f(s) = \frac{-3s^{\alpha-1}}{4} + \frac{\alpha}{2} \pm (\gamma s^\alpha + \sqrt{\frac{\alpha^2}{4} - \frac{12\alpha}{16} + \beta + \frac{9}{16}}) \qquad (\text{for } K_1) \tag{14}$$

$$\pi_f(s) = \frac{-3s^{\alpha-1}}{4} + \frac{\alpha}{2} \pm (\gamma s^\alpha - \sqrt{\frac{\alpha^2}{4} - \frac{12\alpha}{16} + \beta + \frac{9}{16}}) \qquad (\text{for } K_2) \tag{15}$$

To ensure the derivative of the polynomial $\tau_f(s)$ is negative, the appropriate form of the polynomial $\pi_f(s)$ must be selected. Therefore, the most suitable expression for $\pi_f(s)$ is:

$$\pi_f(s) = \frac{-3s^{\alpha-1}}{4} + \frac{\alpha}{2} - (\gamma s^\alpha - \sqrt{\frac{\alpha^2}{4} - \frac{12\alpha}{16} + \beta + \frac{9}{16}}) \tag{16}$$

The function $\tau_f(s)$ is defined as:

$$\tau_f(s) = \tilde{\tau}_f(s) + 2\pi_f(s) = \frac{5}{2} - \alpha + 2\pi_f(s) \tag{17}$$

Substituting the value of $\pi_f(s)$ into $\tau_f(s)$ we can write:

$$\tau_f(s) = 1 - 2\left(\gamma s^\alpha - \sqrt{(\frac{\alpha^2}{4} - \frac{12\alpha}{16} + 16\beta + 9)}\right) \tag{18}$$

Based on the values of $K(s)$ and $\pi_f(s)$, the value of $\lambda(s)$ is obtained as:

$$\lambda(s) = K(s) + D^\alpha \pi_f(s) = [\epsilon - 2\gamma\sqrt{\frac{\alpha^2}{4} - \frac{12\alpha}{16} + \beta + \frac{9}{16}} - \gamma\alpha]s^{\alpha-1} \tag{19}$$

Also

$$\lambda_n(s) = -nD^\alpha\tau(s) - \frac{n(n-1)}{2}D^\alpha D^\alpha \sigma_f(s) = n(2\gamma\alpha s^{\alpha-1}) \tag{20}$$

Using the fact that ($\lambda_n(s) = \lambda(s)$), one obtains:

$$n(2\gamma\alpha s^{\alpha-1}) = \epsilon - 2\gamma\sqrt{\frac{\alpha^2}{4} - \frac{12\alpha}{16} + \beta + \frac{9}{16}} - \gamma\alpha \tag{21}$$

Thus, utilizing the value of γ,β and ϵ , the conformable energy state can be expressed as:

$$E_{nl} = [-2D_e + \sqrt{\frac{D_e}{r_0^2}\frac{\mu}{2\hbar^2}\frac{2\hbar^2}{\mu}}[2\alpha n + \alpha + 2\sqrt{\frac{\alpha^2}{4} - \frac{12\alpha}{16} + D_e r_0^2 + \frac{l(l+1)\hbar^2}{2\mu})\frac{\mu}{2\hbar^2} + \frac{9}{16}}]] \tag{22}$$

For the case of $\alpha = 1$, this result shows good agreement with the literature [33], as clearly demonstrated in the Table **??**, which includes numerical results for the energy states with different values of α. The potential parameters are taken from Ref. [34].

Table 1. Energy states (in eV) of pseudoharmonic potential for N_2,CO molecules with different values of n and l at different values of α.

		N_2				CO			
n	l	$\alpha = 0.2$	$\alpha = 0.5$	$\alpha = 0.8$	$\alpha = 1.0$	$\alpha = 0.2$	$\alpha = 0.5$	$\alpha = 0.8$	$\alpha = 1.0$
0	0	0.02228044	0.05489432	0.08755324	0.10935087	0.036735676	0.086041306	0.135670387	0.168936188
1	0	0.06595773	0.16418266	0.26241458	0.32792754	0.104130339	0.254527961	0.405249027	0.505909491
1	1	0.06649613	0.16468298	0.26291495	0.32842786	0.107724515	0.258122693	0.408844177	0.509504835
2	0	0.10971111	0.27347099	0.43727592	0.54650428	0.171525002	0.423014616	0.674827674	0.842882795
2	1	0.11021143	0.27397132	0.43777624	0.54700453	0.175119173	0.426609348	0.678422839	0.846478145
2	2	0.11121203	0.27497192	0.43877686	0.54800515	0.182302607	0.433793912	0.685608218	0.853663932
3	0	0.15342644	0.38275933	0.61213726	0.76508088	0.238919659	0.591501265	0.944406314	1.179856105
3	1	0.15392676	0.38325966	0.61263757	0.76558121	0.242513836	0.595096003	0.948001471	1.183451449
3	2	0.15492736	0.38426026	0.61363824	0.76658182	0.249697274	0.602280561	0.955186871	1.190637242
3	3	0.15642817	0.38576109	0.61513903	0.76808266	0.260460206	0.613045182	0.965952735	1.201403693
4	0	0.19714177	0.49204767	0.78699859	0.98365755	0.306314323	0.759987929	1.213984967	1.516829415
4	1	0.19764209	0.49254799	0.78749891	0.98415787	0.309908493	0.763582652	1.217580117	1.520424759
4	2	0.19864269	0.49354859	0.78849953	0.98515851	0.317091933	0.770767216	1.224765512	1.527610552
4	3	0.20014353	0.49504943	0.79000037	0.98665933	0.327854869	0.781531837	1.235531375	1.538377003
4	4	0.20214446	0.49705039	0.79200133	0.98866031	0.342182739	0.795861935	1.249863133	1.552709535
5	0	0.24135743	0.60183633	0.96236024	1.20273454	0.373708986	0.928474575	1.483563608	1.853802719
5	1	0.24235803	0.60283692	0.96336087	1.20373516	0.377303156	0.932069307	1.487158758	1.857398069
5	2	0.24385885	0.60433776	0.96486179	1.20523678	0.384486597	0.939253871	1.494344158	1.864583856
5	3	0.24585984	0.60633872	0.96686267	1.20723697	0.395249526	0.950018492	1.505110028	1.875350307
5	4	0.24836073	0.60883967	0.96936647	1.20973795	0.409577396	0.964348593	1.519441784	1.889682839
5	5	0.24836073	0.60883967	0.96936364	1.20973795	0.427450912	0.982224896	1.537320127	1.907562153

The energy states were derived from the special case of the SE for the pseudoharmonic potential strongly depend on the fractional parameter α. When α is assumed to be equal to unity, the results agree with classical quantum mechanical results, which validate the approach used in this study. However, as α decreases, energy levels start to differ significantly, indicating the fractional-order dynamics influence the quantum behavior of the system. Physically, such a transition can be interpreted as a restriction to vibrational motion and hence a decrease in the density of available states. Now, let us determine the corresponding wavefunction for the conformable radial equation. The polynomial solution of the hypergeometric-type function (Rodrigues‘ formula) $y_{nf}(s)$ depends on the determination of the weight function $\rho_f(s)$, as follows:

$$D^{\alpha}[\sigma_f(s)\rho_f(s)] = \tau_f(s)\rho_f(s) \qquad y_{nf} = \frac{B_n}{\rho(s)}\frac{d^n}{ds^n}[\sigma_f^n(s)\rho(s)] \tag{23}$$

And

$$\frac{D^{\alpha}\phi_f(s)}{\phi_f(s)} = \frac{\pi_f(s)}{\sigma_f(s)} \qquad \text{where} \qquad \psi_f(s) = \phi_f(s)y_f(s) \tag{24}$$

By utilizing Eq 24, we obtain:

$$\phi_f(s) = s^{\frac{1}{4}[2\alpha-3+4\sqrt{\frac{\alpha^2}{4}-\frac{12\alpha}{16}+\beta+\frac{9}{16}}]}e^{\frac{-\gamma S^{\alpha}}{\alpha}} \tag{25}$$

and

$$\rho_f(s) = e^{\frac{-2\gamma s^{\alpha}}{\alpha}}[s^{\frac{1}{2}(4\alpha^2-12\alpha+16\beta+9)}] \tag{26}$$

Substituting $\rho_f(s)$ into Eq 23 allows us to obtain the polynomial $y_{nf}(s)$ as follows:

$$y_{nf} = B_n s^{-\sqrt{\alpha^2-3\alpha+64\beta+36}}e^{\frac{2\gamma s^{\alpha}}{\alpha}}\frac{d^n}{ds^n}(s^{n-\sqrt{\alpha^2-3\alpha+64\beta+36}}e^{\frac{-2\gamma s^{\alpha}}{\alpha}}) \tag{27}$$

Using $\psi_f(s) = \phi_f(s)y_{nf}$, the conformable wavefunction can be written as:

$$\psi_f(s) = N_n s^{\frac{1}{4}[2\alpha-3+4\sqrt{\frac{\alpha^2}{4}-\frac{12\alpha}{16}+\beta+\frac{9}{16}}]}e^{\frac{-\gamma s^{\alpha}}{\alpha}}.s^{-\sqrt{\alpha^2-3\alpha+64\beta+36}}e^{\frac{2\gamma s^{\alpha}}{\alpha}}\frac{d^n}{ds^n}(s^{n-\sqrt{\alpha^2-3\alpha+64\beta+36}}e^{\frac{-2\gamma s^{\alpha}}{\alpha}}) \tag{28}$$

For the case of $\alpha = 1$, this result shows exact agreement with the literature [33].

3. CONFORMABLE THERMODYNAMIC PROPERTIES FOR PSEUDOHARMONIC POTENTIAL

To obtain the conformable thermodynamic properties of the Pseudoharmonic Potential, it is important to calculate the vibrational partition function:

$$Z_{vib}(\beta) = \sum_{n=0}^{\lambda} e^{-\beta E_{nl}} \qquad \text{where} \qquad \beta = \frac{1}{K_b T} \tag{29}$$

λ, is the upper-bound vibrational quantum number. At high temperature T (classical limit) the sum can be converted to an integral, and the conformable partition function can be written as:

$$Z_{vib}(\beta) = \int_0^{\lambda} e^{\beta E_{nl}} n^{\alpha-1} dn \tag{30}$$

Using the conformable partition function of equation (30), the other thermodynamic properties such as conformable internal energy U, conformable free energy F, conformable entropy S , and the conformable specific heat capacity C_v can be calculated using the following definitions:

1. **Conformable Internal Energy -** $U(\beta) = -\beta^{1-\alpha}\frac{\partial}{\partial\beta}(lnZ_{vib}(\beta))$
2. **Conformable Free Energy -** $F(\beta) = -\frac{1}{\beta}lnZ_{vib}(\beta))$
3. **Conformable Entropy -** $S(\beta) = K_b\, lnZ_{vib}(\beta) - K_b\beta\beta^{(1-\alpha)}\,\frac{\partial}{\partial\beta}(lnZ_{vib}(\beta))$
4. **Conformable Specific Heat -** $C_v(\beta) = -K_b\beta^2\beta^{(1-\alpha)}\frac{\partial U(\beta)}{\partial\beta}$

For the case of $\alpha = 1$, these definitions are consistent with the well-known thermodynamic definitions in literature.

4. RESULTS AND DISCUSSION

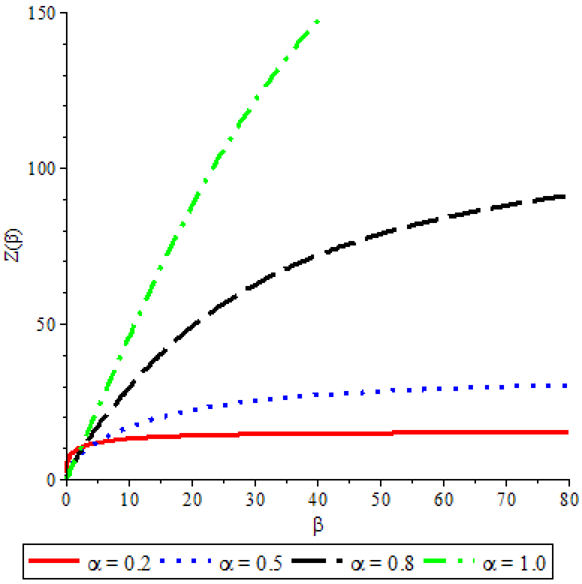

Figure 1. The Conformable Partition function as a function of β for N_2 molecule for different values of α

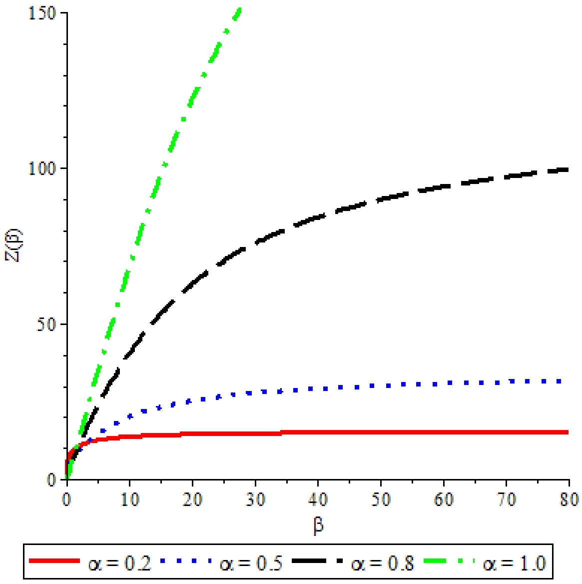

Figure 2. The Conformable Partition function as a function of β for CO molecule for different values of α

The results in Fig. 1 and Fig. 2 represent the behavior of the classical partition function $Z(\beta)$ of the diatomic molecules N_2 and CO, respectively, versus the inverse temperature parameter β, for several values of the fractional parameter α. The calculations of $Z(\beta)$ were performed for four different values of α, namely 0.2, 0.5,0.8, and 1.0, corresponding to different curves. The fractional parameter α strongly affects the partition function. For $\alpha = 1.0$, which corresponds to the classical case, $Z(\beta)$ shows the largest values for all ranges of β. This is the conventional quantum mechanical behavior of the pseudoharmonic potential. When α is varied from 1.0 down to 0.2, the partition functions are strongly suppressed. This suppression is due to the effects of the conformable fractional derivative which changes the energy spectrum and provides a lower density of available states at higher energies. For both diatomic molecules, lower α values result in lower partition functions because certain higher energy states are not thermally accessible. This is important because it shows how conformable derivatives affect the modeling of systems with constrained vibrational dynamics Fig. 1 and Fig. 2 exhibit a similar qualitative dependence of $Z(\beta)$ on α. However, $Z(\beta)$ for CO is always higher compared to N_2, which reflects the different molecular parameters for these diatomic species such as bond strength,

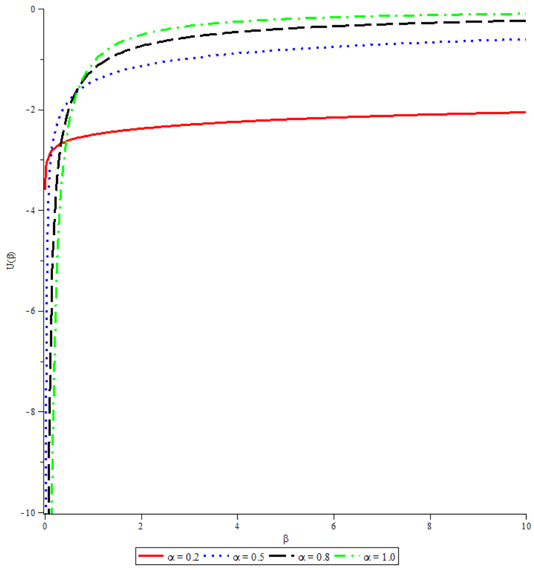

Figure 3. The Conformable Internal Energy as a function of β for N_2 molecule for different values of α.

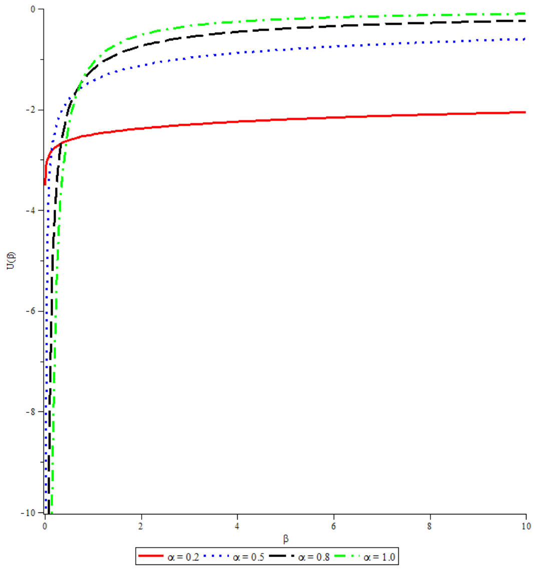

Figure 4. The Conformable Internal Energy as a function of β for CO molecule for different values of α.

reduced mass, and vibrational frequencies. Figures 3 and 4 display the mean vibrational energy $U(\beta)$ versus β for N_2 and CO, respectively. Notice that the energy decreases as β increases and, for all values of α, asymptotically approaches a constant value. For $\alpha = 1.0$, the energy curve starts at the smallest initial value and converges most rapidly, meaning that the system accesses a greater portion of vibrational states than for smaller α values. In contrast, for $\alpha = 0.2$ the energy is higher at the beginning and decays more slowly, reflecting the fact that fractional-order dynamics imposes restrictions on vibrational motion.

Similar trends can also be seen in the mean vibrational energy curves of both molecules; however, CO consistently shows a slightly higher energy value than N_2, especially in the low temperature regime (higher β). These deviations likely result from differences in molecular structure, reduced mass, and vibrational frequencies. Therefore, these results suggest that the influence of the fractional parameter α is modulated by the intrinsic properties of each diatomic molecule. In fact, in systems where vibrational interactions are stronger, more pronounced effects have been observed.

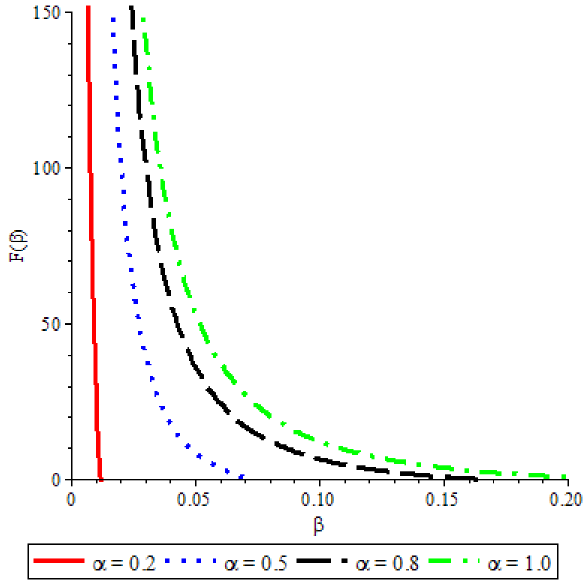

Figure 5. The Conformable Free Energy as a function of β for N_2 molecule for different values of α

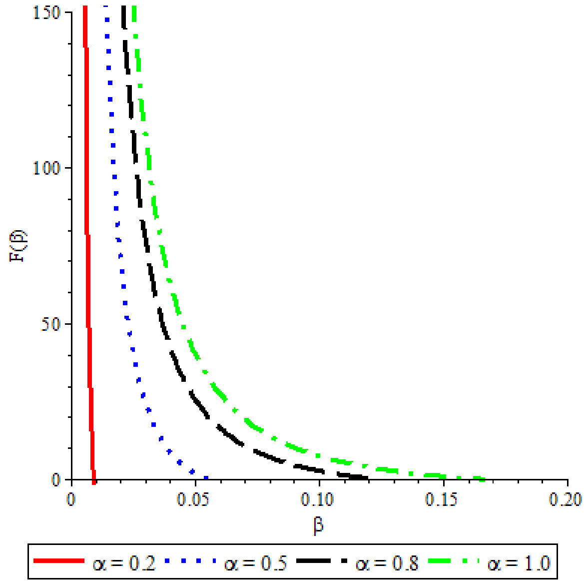

Figure 6. The Conformable Free Energy as a function of β for CO molecule for different values of α

Fig. 5 and Fig. 6 display the dependence of $F(\beta)$ on the β. For $\alpha = 1$, the classical case, $F(\beta)$ decreases rapidly as β increases. This behavior reflects the fact that a higher density of vibrational states is available, resulting in greater thermal stability. As α is lowered, the free energy becomes considerably higher at every given β, this suggesting a lesser ability of the system to minimize its energy. While both the molecules show similar qualitative trends in $F(\beta)$, it is found that CO consistently shows higher values compared to N_2. This reflects the influence of molecular parameters, such as vibrational frequencies and bond strength. CO exhibits stronger vibrational coupling, hence its free energy is elevated compared to N_2, and this effect is much more pronounced for smaller α values. The entropy $S(\beta)$ versus β for N_2 and CO molecules is presented in Figs 7 and 8. For both molecules, the entropy exhibits clear trends related to the fractional order, α. For each molecule, an increase in α in the range from 0.2 to 1.0 results in a decrease in entropy at fixed β, meaning that higher fractional orders restrict the states accessible to the system and thus diminish randomness. At $\alpha = 0.2$, entropy is maximal, reflecting increased flexibility and more accessible states within the system.

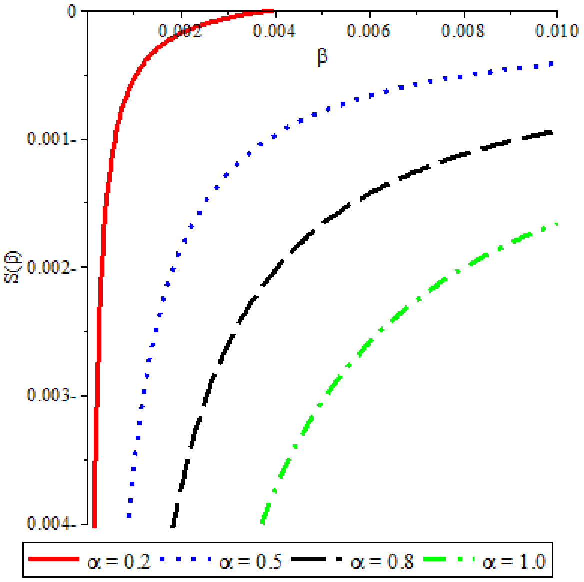

Figure 7. The Thermal Entropy as a function of β for N_2 molecule for different values of α

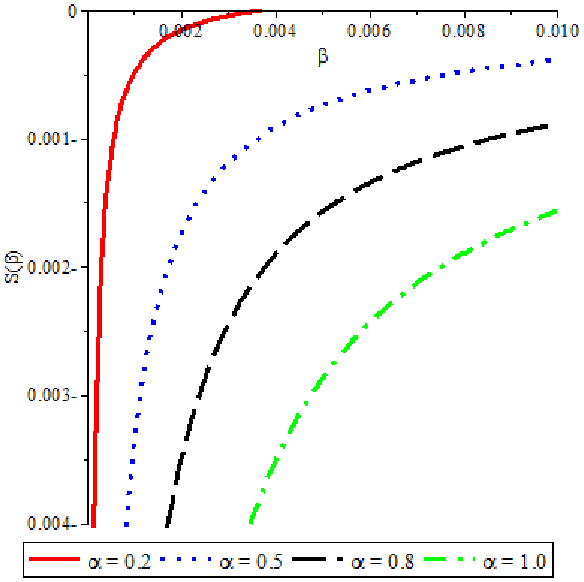

Figure 8. The Thermal Entropy as a function of β for CO molecule for different values of α

Lowering β, which corresponds to a rise in temperature, results in an entropy increase across all α values, in accordance with thermodynamic expectations of increased disorder due to higher temperatures. The limit values of the entropy for small β are found to directly depend on α, reflecting the controlling role that fractional derivatives play in thermodynamics.

Compared to the other molecule, CO has marginally lower entropy than N_2. This is probably due to differences in molecular parameters such as mass or bond stiffness, which affect their quantum states. Finally, the variation of the specific

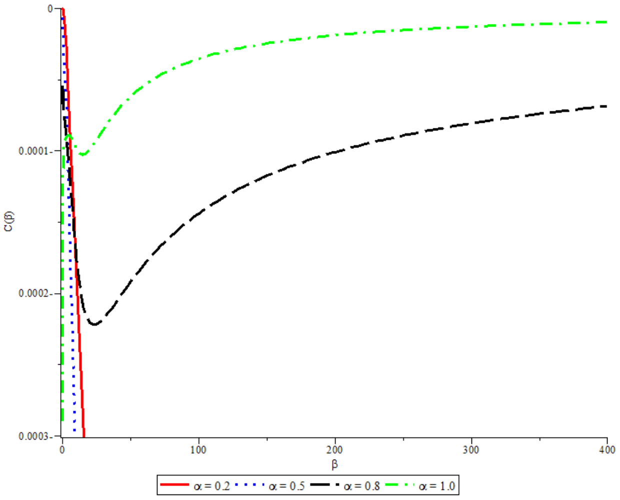

Figure 9. The Conformable Specific Heat as a function of β for N_2 molecule for different values of α

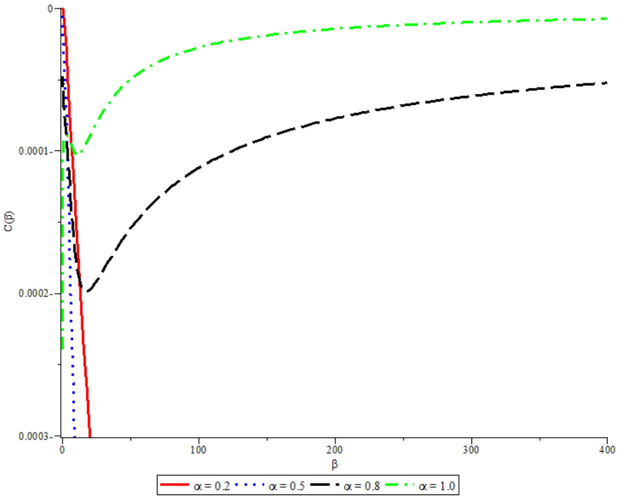

Figure 10. The Conformable Specific Heat as a function of β for CO molecule for different values of α

heat $C(\beta)$ versus β for N_2 and CO molecules clearly shows some interesting features in the thermodynamic behavior of the systems under the influence of fractional calculus. In fact, $C(\beta)$ exhibits different behavior depending on the value of α for both molecules.

For small values of β (high temperatures), the specific heat is small for all α since the system's energy levels are becoming fully populated and saturation effects start to set in. For higher values of β (lower temperatures), the specific heat begins to rise for higher values of α; the largest increase, for $\alpha = 1.0$, begins to dominate for higher values of β. In contrast, lower α values ($\alpha = 0.2$) yield reduced specific heat over the entire range, as expected from a more tightly bound energy distribution because of fractional effects.

When comparing N_2 and CO, the same qualitative trends are observed, but the magnitudes differ slightly; typically, N_2 has marginally higher values of specific heat at large β. This difference may be due to the variation in the molecular properties, such as mass, and vibrational frequencies, which determine the density of states and the energy distribution.

5. CONCLUSIONS

In this paper, the conformable SE with the pseudoharmonic potential was solved using the NU method, considering conformable fractional derivatives. The fractional parameter α played an important role in modifying the energy spectrum and the thermodynamic properties of the molecular systems studied within this framework. Furthermore, using this approach, the energy eigenvalues were analytically obtained and subsequently used to evaluate the classical partition function. Starting from the partition function, important thermodynamic properties, such as conformable internal energy, conformable free energy, conformable entropy, and conformable specific heat have been analyzed for N_2 and CO molecules.

In future work, this approach can be extended to apply the generalized conformable derivative and the NU method to higher-dimensional quantum systems. Although our present study is confined to one-dimensional systems, multidimensional potentials can exhibit a richer behavior. The extension of the methods used here, could potentially provide deeper insight into more complex molecular or solid-state systems.

Conflicts of Interest

The authors declare that there are no conflicts of interest related to the research presented in this manuscript.

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СУМІСНЕ РІВНЯННЯ ШРЕДІНГЕРА З ПСЕВДОГАРМОНІЧНИМ ПОТЕНЦІАЛОМ ТА ЙОГО ТЕРМОДИНАМІЧНІ ВЛАСТИВОСТІ

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У цій роботі метод Нікіфорова-Уварова (NU) використовується для отримання точного розв'язку відповідного радіального рівняння Шредінгера (SE) для псевдогармонічного потенціалу. Ми виводимо як енергетичні стани, так і відповідні хвильові функції, а результати порівнюємо з результатами, описаними в існуючій літературі, для випадку традиційної похідної ($\alpha = 1$). Крім того, отримані енергетичні стани використовуються для розрахунку конформної функції розподілу в класичній границі. Термодинамічні властивості, включаючи конформну вільну енергію Гельмгольца, конформну середню енергію, конформну ентропію та конформну питому теплоємність, обчислюються та аналізуються для молекул N_2 та CO.

Ключові слова: *метод Нікіфорова-Уварова; псевдогармонічний потенціал; термодинамічні властивості; конформна функція розподілу*