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Quantum Information and Energy Spectra Modifications in Diatomic Molecules Due to Topological Defects

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Abstract

Aims: *This study investigates the approximate analytical solutions of the Schrödinger equation for diatomic molecules (NO and CO) in a medium containing topological defects. By employing the Screened Kratzer and Eckart potentials, the research examines how these defects influence energy spectra and quantum information measures, specifically Fisher information and Shannon entropy.*

Method: *The parametric Nikiforov-Uvarov method is applied to obtain bound-state energy eigenvalues and wavefunctions of the Schrödinger equation under the Screened Kratzer-Eckart potential in a defected medium. The study further evaluates quantum information measures, including Fisher information and Shannon entropy, to analyze wavefunction localization. Additionally, the Białynicki-Birula–Mycielski and Stam–Cramér–Rao inequalities are verified to ensure the consistency of computed Shannon entropy and Fisher information entropy values.*

Results: *The findings indicate that topological defects significantly alter energy levels, wavefunction distributions, and quantum information measures in NO and CO molecules. The energy spectra and molecular wavefunctions exhibit notable modifications due to defect-induced distortions. Shannon entropy analysis confirms the uncertainty principle, showing an inverse relationship between position and momentum entropies. Additionally, the satisfaction of the Białynicki-Birula–Mycielski and Stam–Cramér–Rao inequalities further supports the reliability of the entropy and Fisher information results.*

Conclusions: *This study provides valuable insights into the impact of topological defects on quantum properties of diatomic molecules, with significant implications for quantum mechanics, molecular physics, and materials science. The findings contribute to the understanding of energy spectra modifications, wavefunction localization, and quantum information measures in defected media. These results have potential applications in molecular spectroscopy, quantum information theory, and materials engineering, paving the way for further research on molecular systems in complex quantum environments.*

Keywords: Schrödinger Equation, Diatomic Molecules, Topological Defects, Quantum Information, Parametric Nikiforov-Uvarov Method

1. Introduction

Topological defects (TDs) are fundamental phenomena resulting from spontaneous symmetry breaking in various systems, spanning cosmology to condensed matter physics. These defects manifest in forms such as cosmic strings, monopoles, and localized field disruptions [1-3]. In cosmology, TDs likely emerged during early-universe phase transitions, significantly impacting cosmic evolution and structure formation [4-6]. In condensed matter systems, they appear in different forms, including vortices in superconductors, domain walls in magnetic materials, solitons in polymers, and dislocations in liquid crystals [2,7,8]. These defects play a crucial role in shaping the physical properties of materials, affecting electrical conductivity, superfluidity, and the behavior of quantum systems. Their influence extends to fundamental interactions and the structural evolution of the universe [9,10]. Quantum Information Theory (QIT) is an evolving field that merges quantum mechanics with classical information theory to analyze how quantum systems encode, transmit, and process information [11]. Fisher information and Shannon entropy are key concepts in information theory, widely applied in quantum mechanics and statistical physics [12]. In quantum mechanics, Fisher information quantifies the precision of parameter estimation and contributes to the Heisenberg uncertainty principle [13]. Shannon entropy, on the other hand, measures system uncertainty or disorder, providing insight into its informational structure [14]. It is extensively utilized in statistical mechanics to determine system entropy in thermodynamic equilibrium and assess the informational characteristics of quantum states [15]. Diatomic molecules, which consist of two atoms, serve as an essential model for studying quantum phenomena relevant

to QIT [16-20]. Their quantum states can be effectively described using potential models like the screened Kratzer and Eckart potentials, which address vibrational and rotational energy levels, as well as barrier tunneling. The screened Kratzer potential is frequently employed to model diatomic molecular energy levels, while the Eckart potential is particularly significant in quantum tunneling studies. The screened Kratzer potential an extension of the classical Kratzer potential, introduces a screening parameter to account for shielding effects in molecular interactions [21]. When combined with the Eckart potential this hybrid model provides a comprehensive framework for molecular systems, especially in environments with topological defects [22]. This study investigates the relationship between molecular quantum states and information-theoretic measures, including Fisher information and Shannon entropy. Recent research has examined these topics in depth. For instance, Amadi et al analyzed Shannon entropy and Fisher information for H_2 and ScR diatomic molecules using the Deng-Fan-Eckart potential, revealing localization and delocalization patterns in position and momentum spaces while reinforcing uncertainty principles [23]. Similarly, Onate et al solved the Schrödinger equation (SE) for the inversely quadratic Yukawa potential with the parametric Nikiforov-Uvarov (pNU) method and supersymmetric quantum mechanics (SUSYQM), demonstrating the relevance of Shannon entropy as a theoretical tool in consistency with the Heisenberg uncertainty principle [24]. Additionally, Inyang et al employed the Nikiforov-Uvarov method to solve the SE for a combined potential, analyzing Shannon entropy and Fisher information in low-energy states, further validating key entropic inequalities [25]. Omugbe et al explored quantum information measures for an α-deformed Kratzer potential, computing Fisher, Shannon, Rényi and Tsallis entropies, thereby contributing to a deeper understanding of quantum information metrics [26-29]. The impact of topological defects (TDs) on quantum systems has also been extensively investigated. For example, Ikot et al applied the Extended NU method to solve the SE for an exponential-type pseudo-harmonic oscillator in global monopole spacetime, examining the effects of TDs on energy spectra and thermodynamic properties [30]. Similarly, Ahmed et al explored the behavior of quantum particles governed by the SE under a trigonometric Pöschl-Teller potential in the presence of TDs, demonstrating their influence on energy eigenvalues and wave functions relative to flat spacetime [31]. They also calculated Shannon entropy, showing how TDs and potential shape a quantum system's information content. Furthermore, Abu-Shady and Fath-Allah investigated heavy quarkonia in the presence of TDs using the extended Cornell potential and the fractional SE, supported by other related studies [32-40]. Despite extensive research in this area, no study, to the best of our knowledge, has examined the energy spectra of quantum systems in a medium with topological defects while exploring information theory in NO and CO diatomic molecules using the combined Screened Kratzer and Eckart potentials (SKEP). Addressing this gap is the primary motivation for our study. The SKEP takes the form:

$$V(r)=e^{-\varphi r}\left(-\frac{A}{r}+\frac{B}{r^2}\right)+\left(-\frac{w_0}{1-e^{-\varphi r}}+\frac{w_1}{\left(1-e^{-\varphi r}\right)^2}\right)e^{-\varphi r} \tag{1}$$

where $A=2D_e r_e, B=D_e r_e^2$ and D_e is the dissociation energy, and r_e is the bong length. Also, w_0 and w_1 are the strength of the potential, φ is the screening parameter.

1.1 The Theory and Solutions of the Screened Kratzer Plus Eckart Potential With the Topological Defects

The geometry of spacetime corresponding to a point-like global monopole (PGM) is represented by the following line element: [41]

$$ds^2=-c^2dt^2+\frac{dr^2}{\alpha^2}+r^2d\theta^2+r^2\sin^2\theta d\varphi^2 \tag{2}$$

The parameter $0<\alpha=1-8\pi G\eta_0^2<1$ is associated with the global monopole (PGM) and depends on the energy scale. Additionally, Equation (2) represents the spacetime with a scalar curvature.

$$R=R_\mu^\mu=\frac{2\left(1-\alpha^2\right)}{r^2} \tag{3}$$

In this manner, the SE assumes the following form:

$$-\frac{\hbar^2}{2\mu}\nabla_{LB}^2\psi(\vec{r},t)+V(r,t)\psi(\vec{r},t)=i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} \tag{4}$$

The operator $\nabla_{LB}^2=\frac{1}{\sqrt{g}}\partial_i\left(\sqrt{g}g^{ij}\partial_j\right)$ with $g=\det(g_{ij})$ refers to the Laplace-Beltrami operator, $V(rt)= V(r)$ denotes the global monopole potential of order 1. Therefore, the SE for the global monopole (GMP) in a medium containing the point-like global monopole (PGM(1)) takes the form:

$$-\frac{\hbar^2}{2\mu r^2}\left[\alpha^2\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]\psi(r,\theta,\varphi,t)+V\psi(r,\theta,\varphi,t)=i\hbar\frac{\partial\psi(r,\theta,\varphi,t)}{\partial t} \tag{5}$$

Here, we focus on a particular solution to Equation (3), defined in terms of the eigenvalues of the angular momentum operator $\hat{L}^2$, as given by:

$$\psi(r,\theta,\varphi,t)=e^{-\frac{E_{nl}t}{\hbar}}\frac{U(r)}{r}Y_{l,m}(\theta,\varphi) \tag{6}$$

where $Y_{l,m}(\theta,\varphi)$ are spherical harmonics and $R(r)$ is the radial wave function.

The radial wave equation is derived by substituting Eq. (1) into Eq. (5), resulting in:

$$\frac{d^2\psi_n(r)}{dr^2}+\left[\frac{2\mu}{\alpha^2\hbar^2}\left(E-\left[e^{-\varphi r}\left(-\frac{A}{r}+\frac{B}{r^2}\right)+\left(-\frac{w_0}{1-e^{-\varphi r}}+\frac{w_1}{\left(1-e^{-\varphi r}\right)^2}\right)e^{-\varphi r}\right]\right)-\frac{l(l+1)}{\alpha^2r^2}\right]\psi_n(r)=0 \tag{7}$$

Here, $\psi_n(r)$ represents the eigenfunctions, E_{nl} denotes the energy eigenvalues, μ is the reduced mass of the system, h is the reduced Planck's constant, and r is the inter-nuclear separation.

To address the centrifugal term in Equation (7), the Greene-Aldrich approximation is introduced [42].

This method provides an accurate solution to the centrifugal problem for $\varphi \ll 1$, resulting in the following expression

$$r^{-2}\approx\varphi^2\left(1-e^{-\varphi r}\right)^{-2}. \tag{8}$$

We perform a convenient change of variables by setting $y=e^{-\varphi r}$ and incorporate this ansatz, along with Equation (8), into Equation (7). After some simplifications, the resulting radial equation takes the Schrödinger form, and we obtain:

$$\frac{d^2\psi(y)}{dy^2}+\frac{1-y}{y(1-y)}\frac{d\psi(y)}{dy}+\frac{1}{y^2(1-y)^2}\left[\begin{array}{l}-(\varepsilon+\beta_0+\beta_2)y^2+\\(2\varepsilon+\beta_0-\beta_1+\beta_2-\beta_3)y-(\varepsilon+\gamma)\end{array}\right]\psi(y)=0, \tag{9}$$

where

$$\left.\begin{array}{llll}-\varepsilon=\dfrac{2\mu E_{nl}}{\alpha^2\varphi^2\hbar^2}, & \beta_0=\dfrac{2\mu A}{\varphi\alpha^2\hbar^2}, & \beta_1=\dfrac{2\mu B}{\alpha^2\hbar^2}, & \\ \beta_2=\dfrac{2\mu w_0}{\varphi^2\alpha^2\hbar^2}, & \beta_3=\dfrac{2\mu w_1}{\varphi^2\alpha^2\hbar^2}, & \gamma=\dfrac{l(l+1)}{\alpha^2} & \end{array}\right\}. \tag{10}$$

The energy equation and wave function can be explicitly derived using the parametric Nikiforov-Uvarov (pNU) method, as detailed by Tezcan and Sever [43].

The pNU method is particularly effective due to its simplicity and has provided more accurate solutions for wave equations involving various potential energy functions. According to these authors, the standard equation is expressed as:

$$\psi''(s)+\frac{(x_1-x_2s)}{s(1-x_3s)}\psi'(s)+\frac{1}{s^2(1-x_3s)^2}\left[-p_0s^2+p_1s-p_2\right]\psi(s)=0 \tag{11}$$

By applying Eq. (11), the authors derived the condition for the energy equation along with the associated wave function as:

$$x_2n-(2n+1)x_5+\left[2x_8+n(n+1)\right]x_3+x_7+(2n+1)\sqrt{x_9}+\sqrt{x_8}\left[2\sqrt{x_9}+x_3(2n+1)\right]=0 \tag{12}$$

$$\psi(s)=N_{nl}s^{x_{12}}(1-x_3s)^{-x_{12}-\frac{x_{13}}{x_3}}p_n^{\left(x_{10}-1,\frac{x_{11}}{x_3}-x_{10}-1\right)}(1-2x_3s) \tag{13}$$

The parametric constants in Eqs. (12) and (13) are determined as follows:

$$\left.\begin{array}{l}x_1=x_2=x_3=1, x_4=0.5(1-x_1), x_5=0.5(x_2-2x_3),\\ x_6=x_5^2+p_0, x_7=2x_4x_5-p_1,\\ x_8=x_4^2+p_2, x_9=x_3(x_7+x_3x_8)+x_6,\\ x_{10}=x_1+2x_4+2\sqrt{x_8},\\ x_{11}=x_2-2x_5+2\left(\sqrt{x_9}+x_3\sqrt{x_8}\right),\end{array}\right\}$$

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$$\left.\begin{aligned} x_{12} &= x_4 + \sqrt{x_8}, \\ x_{13} &= x_5 - \left(\sqrt{x_9} + x_3\sqrt{x_8}\right) \end{aligned}\right\} \tag{14}$$

Upon Matching Eq. (9) with Eq. (11), the parametric constants in Eq. (14) take the form:

$$\left.\begin{aligned} &x_1 = x_2 = x_3 = 1, x_4 = 0, x_5 = -0.5, \\ &x_6 = \frac{1}{4} + \varepsilon + \beta_0 + \beta_2, x_7 = -2\varepsilon - \beta_0 + \beta_1 - \beta_2 + \beta_3 \\ &x_8 = \varepsilon + \gamma, x_9 = \frac{1}{4} + \gamma + \beta_1 + \beta_3, \\ &x_{10} = 1 + 2\sqrt{\varepsilon + \gamma}, \\ &x_{11} = 2\left(\sqrt{\frac{1}{4} + \gamma + \beta_1 + \beta_3} + \sqrt{\varepsilon + \gamma}\right), \\ &x_{12} = \sqrt{\varepsilon + \gamma}, \\ &x_{13} = -\frac{1}{2} - \left(\sqrt{\frac{1}{4} + \gamma + \beta_1 + \beta_3} + \sqrt{\varepsilon + \gamma}\right) \end{aligned}\right\} \tag{15}$$

By substituting Eqs. (10) and (15) into Eqs. (12) and (13), respectively, we obtain the energy eigenvalue and the associated wave function expressed as:

$$E_{nl} = \frac{\varphi^2 \hbar^2 \alpha^2 l(l+1)}{2\mu} - \frac{\alpha^2 \varphi^2 \hbar^2}{8\mu} \left[\frac{\left(n + \frac{1}{2} + \sqrt{\left(l+\frac{1}{2}\right)^2 + \frac{2\mu D_e r_e^2}{\alpha^2\hbar^2} + \frac{2\mu w_1}{\varphi^2\alpha^2\hbar^2}} \right)^2 + \frac{2\mu w_1}{\alpha^2\varphi^2\hbar^2} - \frac{2\mu w_0}{\alpha^2\hbar^2\varphi^2} + \frac{4\mu D_e r_e}{\hbar^2\varphi\alpha^2} + \frac{l(l+1)}{\alpha^2}}{n + \frac{1}{2} + \sqrt{\left(l+\frac{1}{2}\right)^2 + \frac{2\mu D_e r_e^2}{\alpha^2\hbar^2} + \frac{2\mu w_1}{\varphi^2\alpha^2\hbar^2}}} \right]^2 . \tag{16}$$

The wave function is obtain as;

$$\psi(s) = N_{nl} s^{\sqrt{\varepsilon+\gamma}} (1-s)^{\frac{1}{2}+\frac{1}{2}\left(\sqrt{\frac{1}{4}+\gamma+\beta_1+\beta_3}+\sqrt{\varepsilon+\gamma}\right)} p_n^{\left(2\sqrt{\varepsilon+\gamma}, 2\sqrt{\frac{1}{4}+\gamma+\beta_1+\beta_3}+\sqrt{\varepsilon+\gamma}\right)}(1-2s) \tag{17}$$

where N is normalization constant and can be evaluated using Eq.(18)

$$\int_0^\infty |\psi_{nm}(\gamma)|^2 \, dr = 1 \tag{18}$$

1.2 Shannon entropy

The Shannon entropy, representing logarithmic probability density, offers insights into a system's probability distribution [44].

$$S(\rho_{nl}) = -\int \rho_{nl}(r) \ln \rho_{nl}(r) dr \tag{19}$$

and

$$S(\gamma_{nl}) = -\int \gamma_{nl}(p) \ln \gamma_{nl}(p) dp \ , \tag{20}$$

Here, $S(\rho_{nl})$ represents the position space Shannon entropy, and $S(\gamma_{nl})$ denotes the momentum space Shannon entropy. The probability densities (PD) in the position and momentum spaces are specified in Eq. (21) and Eq. (22), respectively.

$$\rho_{nl}(r) = |\psi(r)|^2 \tag{21}$$

and

$$\gamma_{nl}(p) = |\psi(p)|^2 \tag{22}$$

$\psi(p)$ represents the momentum-space wave function, obtained by applying the Fourier transform (FT) tov $\psi(r)$ .The Berkner, Bialynicki-Birula, and Mycieslki (BBM) [45]. Investigated this concept by establishing an entropic link between position and momentum spaces (PMS) through Shannon entropy, denoted as $S(\rho_{nl}) + S(\gamma_{nl}) \geq D(1+\ln\pi)$, where D indicates the number of spatial dimensions.

1. 3 Fisher information

In contrast, Fisher Information is a local measure of information entropy, factoring in differential components that make it sensitive to local variations in probability density. Recognized as a fundamental measure of information entropy, it is vital in determining the localization of probability densities. Additionally, Fisher information can be viewed as a measure of the oscillator's degree, relevant in quantum mechanical kinetic energy calculations. It is expressed in both position and momentum spaces as [46]:

$$I(\rho)=\int \frac{\left|\nabla \rho_{nl}(r)\right|^2}{\rho_{nl}(r)}dr \tag{23}$$

$$I(\gamma)=\int \frac{\left|\nabla \rho_{nl}(p)\right|^2}{\rho_{nl}(p)}dp \quad . \tag{24}$$

In Fisher information theory, higher Fisher information indicates better precision in predicting the system's localization, leading to increased fluctuations. For any central potential model with an arbitrary angular momentum quantum number lll, the product of Fisher information in both position and momentum spaces must comply with the Stam-Cramér-Rao inequality [47,48]

$$I(\rho)I(\gamma)\geq 9\left[2-\frac{2l+1}{l(l+1)}|m|\right]^2\geq 36 \tag{25}$$

2. Results and Discussion

This study explores the approximate analytical solutions of the Schrödinger Equation (SE) for the diatomic molecules nitric oxide (NO) and carbon monoxide (CO) using the SKEP approach. These molecules were chosen due to their critical roles in chemical synthesis, bonding characteristics, thermal stability, and electronic transport properties. The spectroscopic parameters used in this analysis were sourced from previous studies (Ref. [50]) and are presented in Table 1. They were adapted using the conversion method detailed in Ref. [49]. NO and CO are significant across industrial, environmental, and biological domains. CO plays a crucial role in metal refining, fuel synthesis, and atmospheric chemistry, affecting combustion dynamics and pollutant formation. NO is vital in biological signaling pathways, catalytic processes, and environmental chemistry, particularly in air pollution and nitrogen cycle reactions. Investigating their quantum mechanical properties enhances our understanding of their stability, reactivity, and interaction mechanisms. This knowledge is essential for advancing applications in material science, atmospheric modeling, and molecular spectroscopy, contributing to innovative technologies and improved environmental management strategies. Table 2 illustrates the energy spectra of CO and NO across different quantum states (1s, 2s, 2p, 3s, 3p) for various values of the topological defect parameter (α = 0.3, 0.6, 0.9, and 1.0). When α = 1.0, no topological defect is present, and the energy levels remain unchanged. However, as α increase from 0.3 to 0.9, the energy levels shift, demonstrating the significant influence of the topological defect on molecular states. For both CO and NO, lower defect parameter values may distort electronic structures, altering bonding characteristics and molecular stability. This impact is likely more pronounced in higher energy states, where electron distributions are more sensitive to topological variations. Consequently, molecular properties such as dipole moments, reactivity, and spectral transitions could be affected under defected conditions. The differences in response between CO and NO could stem from their distinct electronic configurations and bond orders. CO, a stable molecule with a triple bond, may exhibit different sensitivity to defects than NO, which has an unpaired electron. Understanding these effects is crucial in material science, nanotechnology, and quantum chemistry, where defects influence molecular interactions and electronic properties. Tables 3 and 4 present the Shannon entropy and Fisher information for CO and NO in their ground states. Shannon entropy quantifies the uncertainty or spread of the probability distribution, increasing from 5.20991 to 5.22009 for CO while slightly decreasing from 2.27308 to 2.27208 for NO. This indicates a more delocalized electron cloud for CO. Fisher information, which measures localization, increases from 53.20159 to 54.06868 for CO and decreases from 45.30873 to 44.53173 for NO. This suggests that CO's electronic density becomes more localized, whereas NO exhibits slight delocalization. In molecular physics, higher entropy and lower Fisher information correlate with greater delocalization, influencing chemical reactivity and bonding. CO's localized density implies stronger bonding, while NO's behavior reflects its paramagnetic nature and reactivity, which are significant in atmospheric and biological processes. Figures 1 and 2 illustrate the wavefunction and probability density distributions of CO and NO as functions of position for different principal quantum numbers. In quantum mechanics, the wavefunction describes a system's quantum state, while its square modulus represents the probability density of finding a particle at a given position. Figures 1(a) and 2(a) show wavefunction oscillations corresponding to quantized energy levels, which increase in complexity with higher quantum numbers. This behavior is typical of bound states in a potential well, where the number of nodes (zero crossings) corresponds to the quantum number. Figures 1(b) and 2(b) depict the probability density, which is essential for understanding the likelihood of finding the molecule at specific positions. Higher probability densities indicate favored spatial locations due to quantum confinement. Differences in CO and NO distributions arise from molecular mass, bond potential, and electron distribution variations. These results physically illustrate how quantum confinement influences molecular behavior. The differences between CO and NO wavefunctions highlight their

distinct electronic structures, which impact spectroscopic transitions, reaction dynamics, and molecular interactions. These insights are crucial for applications in atmospheric chemistry, catalysis, and molecular spectroscopy.

Table1: Spectroscopic Data for the Diatomic Molecules Chosen in this Study [50]

Molecules	$D_e(eV)$	$\alpha^{-9}\left(A^{-1}\right)$	$r_e(\text{Å})$	$\mu(MeV)$
CO	11.225600000	2.29940	1.1283	0.63906749030
NO	8.0437300000	1.86430	1.1508	5.91053826200

Table 2: Energy Spectra of CO and NO Molecules Across Different Quantum States for Varying Values of the Topological Defect Parameter

State	α	CO	NO
1s	0.3	−6.120956	−62.37689
	0.6	−6.008354	−62.21348
	0.9	−5.897034	−62.05044
	1.0	−5.860211	−61.99618
2s	0.3	−6.04576	−62.26792
	0.6	−5.86029	−61.99622
	0.9	−5.67839	−61.72559
	1.0	−5.61855	−61.63562
2p	0.3	−6.04452	−62.26758
	0.6	−5.85791	−61.99568
	0.9	−5.67412	−61.72469
	1.0	−5.61347	−61.634574
3s	0.3	−5.97115	−62.15912
	0.6	−5.71453	−61.77966
	0.9	−5.46487	−61.40230
	1.0	−5.38318	−61.27697
3p	0.3	−5.96992	−62.15878
	0.6	−5.71217	−61.77911
	0.9	−5.46063	−61.40140
	1.0	−5.37815	−61.27592

Table 3: Shannon Entropy for the Diatomic Molecules in Their Ground State

	CO			NO		
φ	S_γ	S_p	$S_T \geq 2.14473$	S_γ	S_p	$S_T \geq 2.14473$
0.1	1.52710	3.68281	5.20991	0.01836	2.25472	2.27308
0.2	1.52838	3.68406	5.21244	0.01561	2.25721	2.27282
0.3	1.52966	3.68533	5.21499	0.01288	2.25970	2.27258
0.4	1.53095	3.68659	5.21754	0.01015	2.26217	2.27232
0.5	1.53223	3.68786	5.22009	0.00744	2.26464	2.27208

Table 4: Fisher Information for the Diatomic Molecules in Their Ground State

	CO			NO		
φ	I_γ	I_p	$I_\gamma I_p \geq 4$	I_γ	I_p	$I_\gamma I_p \geq 4$
0.1	4042.34372	0.01316	53.20159	2109.95172	0.02149	45.30873
0.2	4063.00349	0.01314	53.41931	2115.06310	0.02137	45.21822
0.3	4083.78457	0.01311	53.63646	2117.17525	0.02126	45.01772
0.4	4104.68789	0.01308	53.85291	2118.28818	0.02114	44.77227
0.5	4125.71443	0.01305	54.06868	2119.40189	0.02103	44.53173

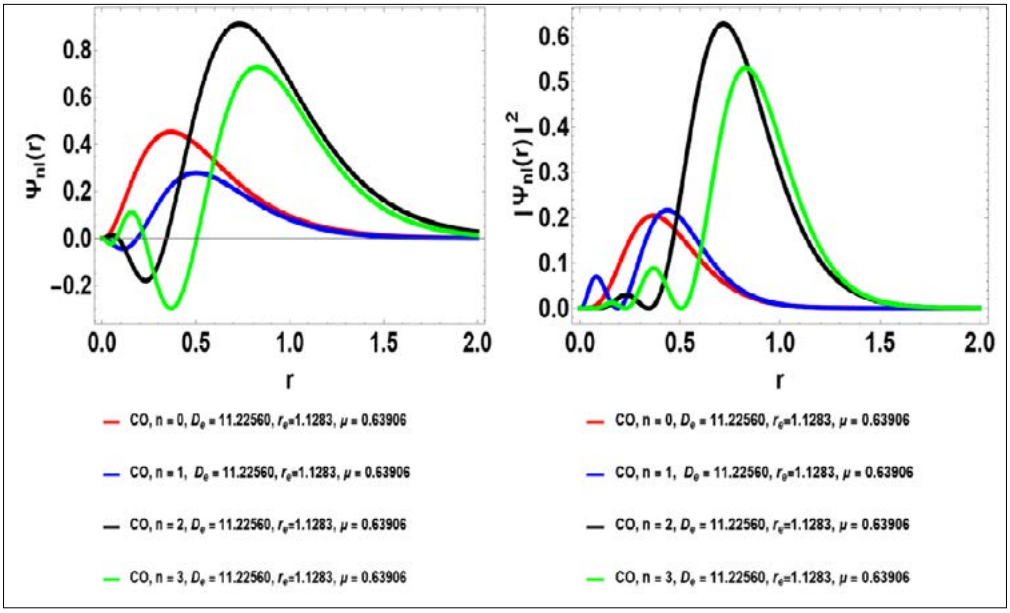

Figure 1: (a, b): The Wave Function and the Probability Density for CO as a Function of Position for Various Principal Quantum Numbers

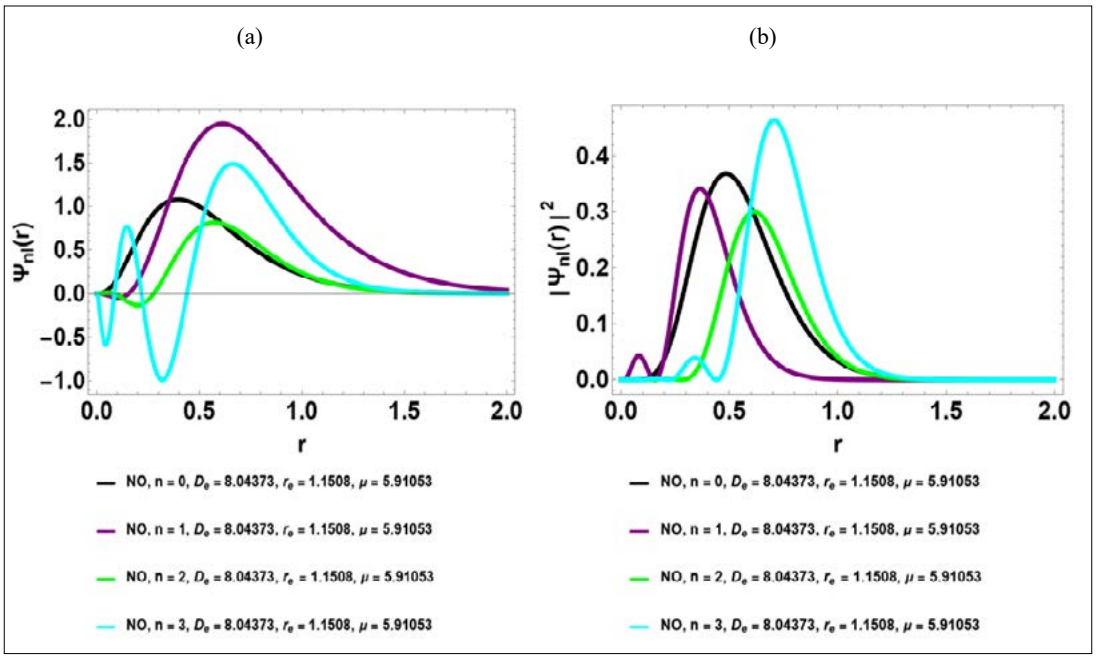

Figure 2: (a,b): The Wave Function and the Probability Density for NO as a Function of Position for Various Principal Quantum Numbers

3. Conclusion

This study provides an analysis of the effects of topological defects on the quantum states of diatomic molecules, specifically CO and NO, using the Screened Kratzer and Eckart Potentials (SKEP). The analytical solutions of the Schrödinger equation obtained via the parametric Nikiforov-Uvarov method offer a clear understanding of how defect parameters influence molecular energy spectra and quantum information measures. The results demonstrate that decreasing the defect parameter leads to significant alterations in energy levels, suggesting changes in molecular stability and electronic distributions. Additionally, the variations in Fisher information and Shannon entropy highlight the role of topological defects in localizing or delocalizing electronic density, which has implications for molecular reactivity and spectroscopic transitions. These findings contribute to the broader understanding of defect-induced quantum effects in molecular and material sciences. It was discovered that the Bialynicki, Birula and Mycielski and Stam-Cramer-Rao inequalities for Shannon entropy and Fisher Information entropies respectively were satisfied. Future research could extend these insights by exploring additional diatomic molecules, employing numerical simulations, and considering more complex potential models to further unravel the influence of topological defects on quantum systems.

Availability of Data and Materials
All data generated during this study are fully referenced within the paper.

Competing Interests
The author declares no conflicts of interest.

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Author Contribution
E.P.I prepared the original draft and validated the results.

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