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Analysis of Information Entropies for He-Like Ions

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Abstract

The electronic structure, a special quality of an atomic or molecular system, is the major factor for further realization of physical results. However, in this paper, we present the topical issue of normalized electron density in position and momentum spaces, Shannon, Rényi, and Tsallis entropies to quantify the reach of electron delocalization for several atomic systems. Hartree-Fock-Roothaan (HFR) wave function is performed and considered for He-like ions using single-Zeta β-type orbital (βTOs) basis set to investigate the affecting of electron density and information entropies. The electron density maxima in position space are raised, and their positions move toward the nucleus as Z increases, in accordance with the increasing attractive force of the nucleus, and vice versa in momentum space. Shannon's entropy has impacted the delocalization of the electron in different atomic systems. In the limit $\gamma \to 1$, both Rényi and Tsallis entropy results recover Shannon's entropy value. Rényi and Tsallis entropies decrease by increasing γ. Indeed, the estimated results have been calculated via the Wolfram Mathematica program and have good agreement with the literature results. The obtained results may be a useful reference for future studies on theoretical information quantities.

Keywords:

Shannon; Rényi;
Tsallis Entropies;
Hartree-Fock-Roothaan;
Helium-Isoelectronic Series;
β-type Orbitals.

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1- Introduction

The Shannon, Rényi, and Tsallis entropies have described an enormous and interesting field in atomic and molecular structures, whereas their applications paved the way for extensive studies of a wide range in various quantum mechanical systems [1-11]. Shannon's entropy reveals changes in the radial density function and has focused on quantifying the uncertainty of random variables as well as the localization or delocalization of electronic systems. Rényi's entropy discussed quantum entanglement [12–15]. Tsallis' statistics are demonstrated in ultra-cold quantum gases [16, 17]. Furthermore, Shannon's entropy in both position and momentum spaces has been presented with the Schrödinger equation and the Kratzer potential [18, 19]. Shannon's entropy for helium atoms has been calculated numerically by considering the Kinoshita type wave function [20, 21]. The Shannon entropy in position space has investigated the electron correlation effects using correlated Hylleraas wave functions [22–24].

Indeed, Shannon entropy in position and momentum eigenstates was accounted for by a simple density functional theory (DFT) method and radial Kohn-Sham equation for He-like ions and showed excellent agreement with the Hartree-Fock framework [25]. The values of entropy were extended for ground [26] and excited [27] states using the correlated Hylleraas wave function. The information entropies have been studied numerically and analytically by considering the Rydberg quantum hydrogenic states [28, 29]. In addition, these entropies were investigated for neutral atoms and molecules within the density functional reactivity theory framework [30]. Shannon and Rényi entropies were investigated for helium atoms in both ground and excited states using correlated and uncorrelated wave functions [22, 27, 31]. These entropies were modified for H-atom [32] in terms of Fisher-Rényi's product and generalized statistical complexity. The discontinuity of entropies is shown and calculated in Shi & Kais (2004, 2005) [33, 34] by solving

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Hyllerase-type wave functions for He-like ions. By using different wave functions, the entropies can be well described by the exponential Coulomb-potential [35–37], the combination of Yukawa and exponential-Coulomb potentials [38], or concerning Morse potential [39]. This paper studies the information entropies of $1s^2$-state atomic systems in position and momentum spaces. It is illustrated that HFR is based on single-Zeta βTOs [40]. The paper is arranged as follows: Typically, it discusses the theoretical background of the wave function and information entropies in Section two. Section three discusses the findings obtained using the radial density function basis set and accurately compares them to the literature. Finally, Section four summarizes and concludes the findings.

2- Research Methodology

Figure 1 shows the flowchart of the research methodology through which the objectives of this study were achieved.

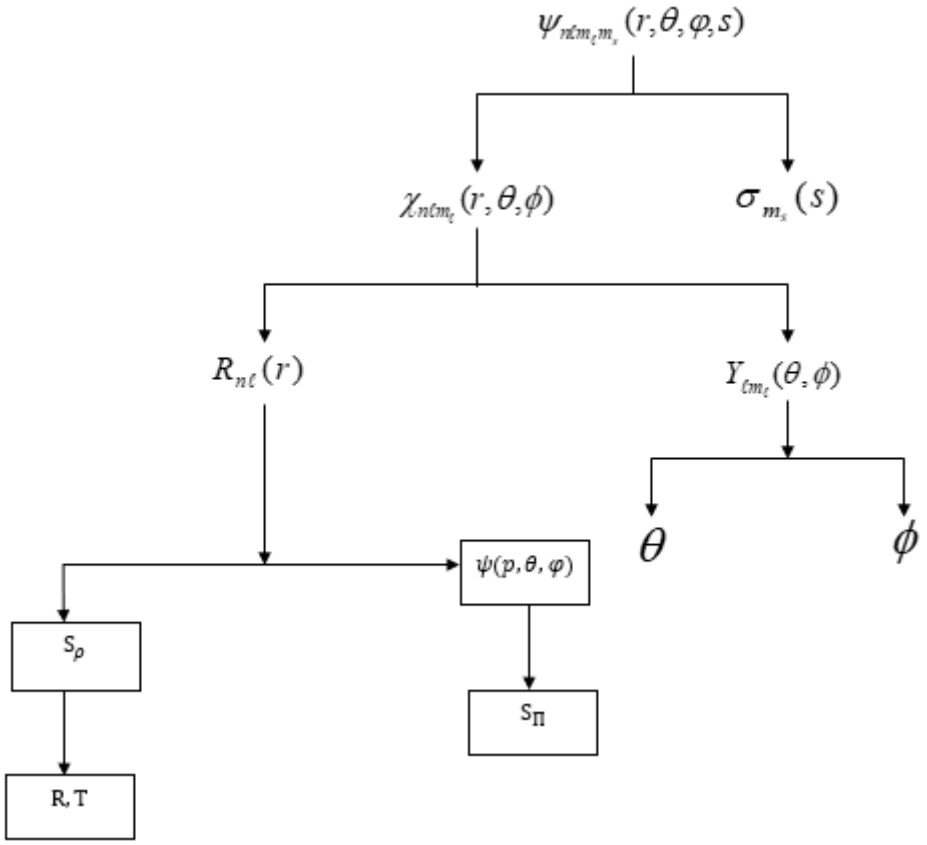

Figure 1. Flow chart of research methodology

2-1- Wave Function

The nonrelativistic Hamiltonian of $1s^2$-state is:

$$H = -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} \quad (1)$$

r_1 and r_2 are the electrons-nucleus distance, $r_{12}$is the interelectronic separation, $\nabla^2_{1,2}$ corresponds to the kinetic energy of each electron, Z/r_{12} denote the potential attraction energy with Z is the nuclear charge, and $1/r_{12}$ represents the interelectronic repulsion energy. Equation 1 includes a boundary that denotes the repulsion between electrons, however, Schrödinger equation cannot be solved exactly. Hence, Slater determinant is mentioned to describe the wave function of independent particles [41] and solve Equation 1:

$$\Psi_{HF} = |\psi_1(x_1)\psi_2(x_2)\ldots\psi_N(x_N)\rangle \quad (2)$$

with $\psi_1(\vec{x}_i)$ is the components of spin-radial and angular co-ordinate wave function in position space and defined as some set of analytic basis functions:

$$\psi_1(\vec{x}_i) = \sum_{i=1}^{j} C^i_{nlm}\chi_{nlm}\, s(\delta) \quad (3)$$

The constant-coefficient $C^i{}_{nlm}$ is determined by minimizing the energy, while the basis function χ_{nlm} corresponds to the normalized βTOs which is the picture of a linear combination of STOs [40, 42–45]:

$$\chi_{q,l}^{m}(\alpha;r,\theta,\varphi) = Nr^{l}Y_{l}^{m}(\theta,\varphi)\mathcal{R}(\alpha r) \quad (4)$$

The factor N represents the normalization of the radial part:

$$N = \frac{2^{l+q}\alpha^{l+1}}{(l+q)!}\sqrt{\frac{\alpha\,\Gamma(2l+2q+2)\,l!\,\Gamma(l+2q)}{\Gamma(2l+4q)\Gamma(2l+1)}} \quad (5)$$

$\Gamma(x)$ is he gamma function. $Y_{l}^{m}(\theta,\varphi)$ is the wave function angular part:

$$Y_{l}^{m}(\theta,\varphi) = P_{l|m|}\Theta_{m}(\varphi) \quad (6)$$

Here $P_{l|m|}$is the associated Legendre function. Furthermore, if spherical harmonics are complex [46], then $\Theta_{m}(\varphi)$ has the form as:

$$\Theta_{m}(\varphi) = \frac{e^{im\varphi}}{\sqrt{2\,\pi}} \quad (7)$$

On the other hand, for real spherical harmonics, $\Theta_{m}(\varphi)$ has written as follow as:

$$\Theta_{m}(\varphi) = \frac{1}{\sqrt{\pi(1+\delta_{m0})}}\begin{cases}\cos|m|\varphi, & \text{for m } \geq 0\\ \sin|m|\varphi, & \text{for } m < 0\end{cases} \quad (8)$$

The radial part of the wave function R(r) is described via reduced Bessel function [40, 42] with an integer $q \geq 1$, yielding;

$$\mathcal{R}(\alpha r) = e^{-\alpha r}\sum_{i=0}^{q-1}\frac{\Gamma(q+i)(\alpha r)^{q-i-1}}{\Gamma(q-i)\,i!2^{i}} \quad (9)$$

It is shown that βTOs have the form of a linear combination of STOs [40, 42] "due to the simplicity of their Fourier transforms enables to approximate two-center distributions by a sum of one-center distributions placed at the line connecting the original two-centers" [40, 47]. The momentum-space wave function is calculated by a Fourier transform. It is the radial part of the momentum space wave function which is related to the radial part of the position space wave function by a spherical Bessel transform of Equation 3.

2-2- Shannon, Rényi, and Tsallis Entropies

In this work, Shannon S, Rényi R_{γ}, and Tsallis T_{γ} entropies of order γ were studied. The quantities emerged from information theory and probability in position and momentum spaces, extended by considering normalized electron density $\rho(\vec{r})$ of wave function $\psi(\vec{r},\vec{x}_{2},\ldots,\vec{x}_{N}$, yielding;

$$\rho(\vec{r}) = |\psi(\vec{r},\vec{x}_{2},\ldots,\vec{x}_{N}|^{2}ds_{1}\,d\theta_{1}d\varphi_{1}d\vec{x}_{2},\ldots,\vec{x}_{N} \quad (11\text{-a})$$

$$\Pi(\vec{p}) = |\psi(\vec{p},\vec{x}_{2},\ldots,\vec{x}_{N}|^{2}ds_{1}\,d\theta_{1}d\varphi_{1}d\vec{x}_{2},\ldots,\vec{x}_{N} \quad (11\text{-b})$$

Where $\vec{x}_{i}$ is the spin $\vec{s}_{i}$ and space-coordinate of the i_{th} electron, $\vec{r} = (r_{i},\theta_{i},\varphi_{i})$. For position and momentum spaces, Shannon's entropy for the N-electron system is realized [1, 48]:

$$S_{\rho} = -\int_{0}^{\infty}\rho(\vec{r})\;ln\;\rho(\vec{r})\;4\pi r^{2}d\vec{r} \quad (12\text{-a})$$

$$S_{\Pi} = -\int_{0}^{\infty}\Pi(\vec{p})\;ln\;\Pi(\vec{p})\;4\pi p^{2}d\vec{p} \quad (12\text{-b})$$

The electron density of momentum-space $\Pi(\vec{p})$ is described by Equation 10. For any 3-dimensional system, the Bialynicki-Birula and Mycielski (BBM) uncertainty relation or localization is given by [49]:

$$S_{\rho} + S_{\Pi} \geq 3(1 + ln\,\pi) \quad (13)$$

Smaller (larger) values of the entropies are related to the underlying densities of localization (delocalization), respectively.

Rényi entropy is written as:

$$R_{\rho}(\gamma) = \frac{1}{1-\gamma}\;ln\left(\int_{0}^{\infty}\rho(\vec{r})^{\gamma}\,4\pi r^{2}d\vec{r}\right) \quad (14)$$

The index γ≠1. Generally, Equation 12 is the limit of Equation 14 for $\gamma \to 1$. However, Equations 12 and 14 are alternative. Indeed, at $\gamma \to 1$, Equation 14 can be calculated analytically by using the *L'Hôpital's* rule or calculated numerically by considering γ close to 1.

Tsallis entropy has formed as follow:

$$T_\rho(\gamma) = \frac{1}{\gamma-1}\left(1 - \int_0^\infty \rho(\vec{r})^\gamma \, 4\pi r^2 d\vec{r}\right) \quad (15)$$

The constrains, γ is a real number and it is utilized as an appropriate variable in the status of systems that are not realized sufficiently [50]. In the limit $\gamma \to 1$, Equation 15 turns out collective and reduces to Equation 12 that recovers the Boltzmann Gibbs statistics [1].

3- Results and Discussion

The electron density, information entropies in the case of some atomic system ($2 \leq Z \leq 10$) (different solid color curves) was examined. HFR wave function was discussed and was tested by a single Zeta βTOs basis set. The HFR wave function issues reasonable values for the physical quantities at high Z. Figure 2-a illustrated the electron probability in position space at distance r from the atom center for ($2 \leq Z \leq 10$) atomic system. The electron density maxima are raised, and their positions move toward the nucleus as Z increases, in terms of increasing the attractive force of the nucleus. Indeed, Figure 2-b mentions the positions of the maxima in the radial electron probability density in momentum space shift to larger p with increasing Z, paralleling the rise in the electron's kinetic energy. This was evident when one realizes that nearest to the nucleus the electron possesses small potential energy and large kinetic energy, while far away the status is reversed [51].

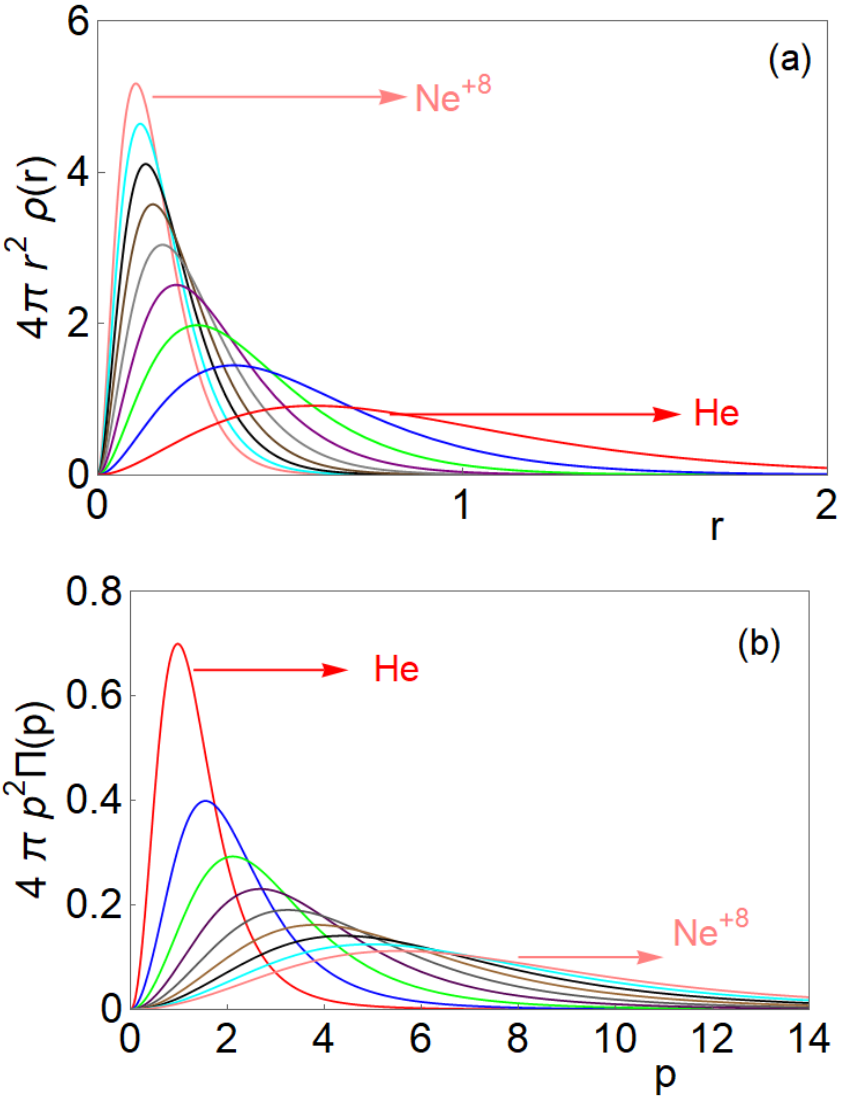

Figure 2. Electron density function; (a) Position and, (b) Momentum spaces Equation 11 of $1s^2$ state of Helium-isoelectronic series

Figure 3 shows $S\rho$ Equation 12-a derive from core and valence areas in the system, respectively, for ($2 \leq Z \leq 10$) atomic system. In Figure 3-a (red curve), it was noticed that tiny peak for He atom (red curve) close r=0 according to localization of the density distribution urged by the Coulomb potential. On the other hand, in Figures 3-b and 3-c, for large Z, a clear positive peak is increasing as well as the regions under the curves over r-axis are largest than under r-axis. The impact of charge influences and leads to focus the charge density distribution on the core region. Indeed, the

repulsion between electrons in the valence region makes the electron density delocalized. The interchange of S_ρ concerning the size of the basis set is demonstrated. S_ρ of He and Li^+ accumulate preferably due to the extra dense distribution of the wave functions. The finding results have been compared to those in Saha et al. [52] and agreed for higher Z than for smaller Z values.

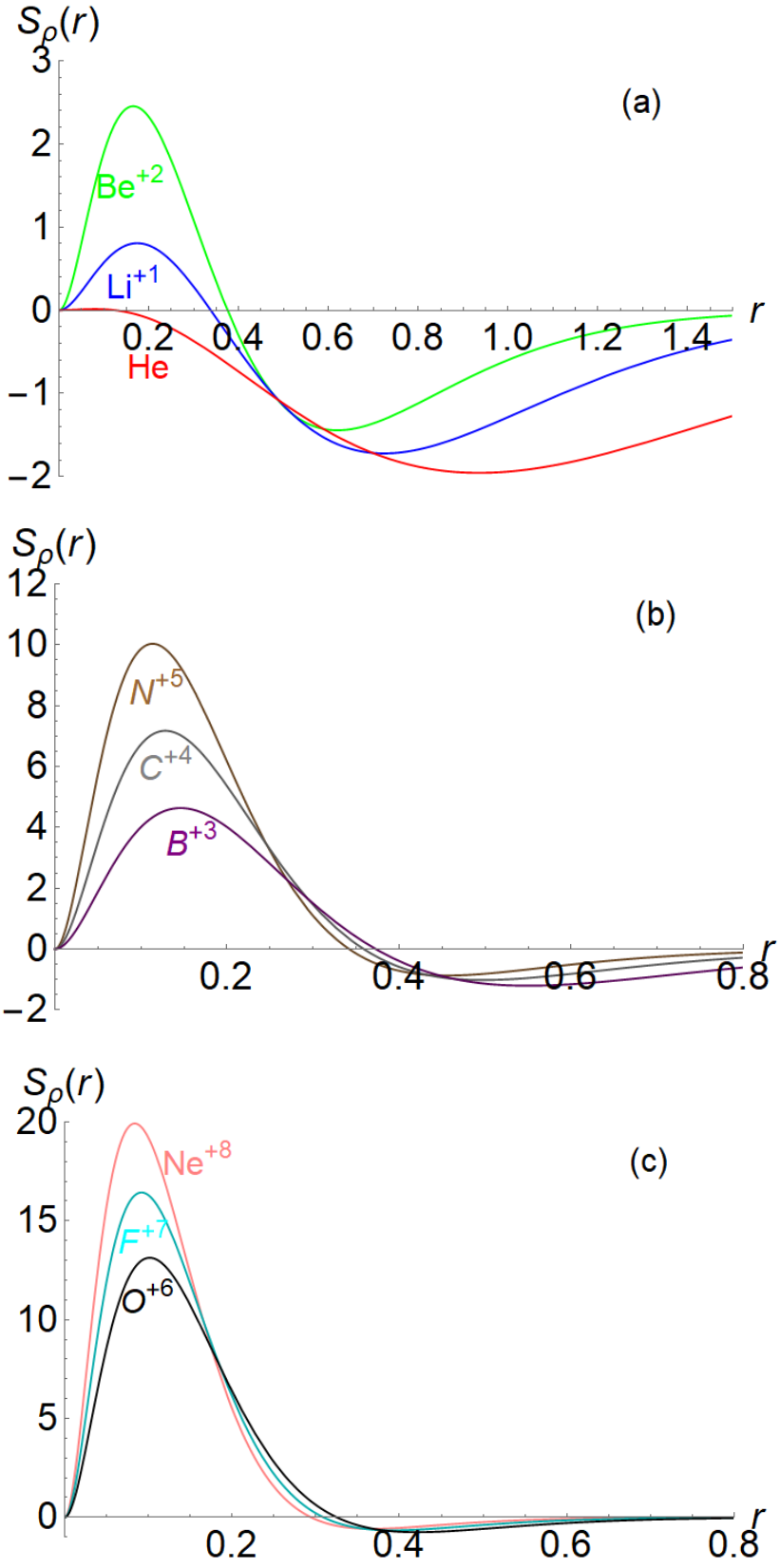

Figure 3. (a), (b), and (c) show Shannon entropy S_ρ in position space Equation 12-a versus r for $1s^2$ state of Helium-isoelectronic series

In momentum space, S_Π in Figure 4 is negative for all p values and the curve is a bit compressed due to the interaction between electrons progressively reducing and attractive interaction between electron and nucleus is increased at high Z atoms. Our Shannon entropy results have good agreement above to 3-digit Z=2 and rise to 4 digits at high atomic numbers in comparison to the literature [7, 33, 35, 52].

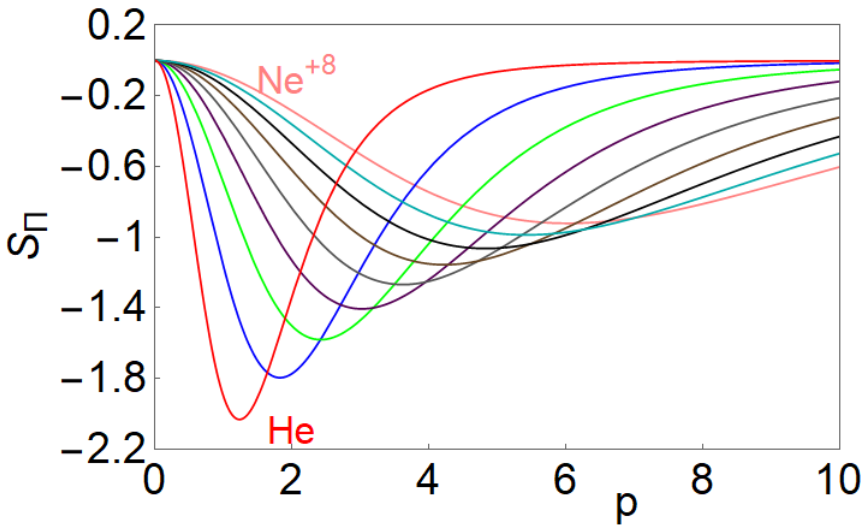

Figure 4. Shannon entropy S_Π in momentum space versus *p*for $1s^2$ state of Helium-isoelectronic series

Liu et al. [30] has been shown the sub-additivity of N-electron S_ρ has the form as

$$S[|\psi(\vec{r},\vec{x}_2,\ldots,\vec{x}_N|^2] \leq 2S_\rho(r) \tag{16}$$

The inequality turns on to a Hartree-Fock wave function result, which means the electrons are uncorrelated and independent [30, 53]. Equation 16 is practical by comparing S_ρ in terms of different densities. Indeed, Figure 3 shows that S_ρ charge density is quite negative with a maximum value of $S_\rho = 5.1410$ which obtained by the subadditivity of S_ρ Equation 16 which look likes to be acceptable according to $2 \times 2.57499 = 5.1410$, and density is delocalized. In the case of $Z = 4$, the charge density of S_ρ is positive and has a large area and density localizes with S_ρ=0.5140, whereas for $Z = 5$, the charge density of S_ρ is positive and further localized but the sign of S_ρ is changed which is linked to the overturn charge density of S_ρ. In general, the flipping values have acceptable for realizing the charge density localization, i.e., the distribution $\rho(r)$ is further localized which refers to a small value of S_ρ, and vice versa. BBM formula Equation 16 has been discussed in Table 1. S_ρ calculates the uncertainty localization of the particle in space. The entropy in position space decreases via increasing Z while the entropy in momentum space increases. Thus, as the attractive nuclear interaction increases, the position space density localizes while the momentum space density delocalizes, as the kinetic energy increases. The uncertainty has tiny and the localization accuracy of the particle is higher in position space predicting. Similarly, S_Π determines the uncertainty of the particle in momentum. The entropies obtained individually decrease without restriction when the identical probability density is being more and more concentrated, i.e., when S_ρ is increasing. The restriction from the sum of two entropies denotes that the overall uncertainty in position and momentum cannot be less than Equation 16.

Table 1. Position and momentum spaces entropies of $1s^2$ state of Helium-isoelectronic series

Atom	S_ρ	S_Π	$S_\rho + S_\Pi$
He	2.57499	3.99161	6.56659
Li^{+1}	1.19351	5.37526	6.56877
Be^{+2}	0.257001	6.31096	6.56796
B^{+3}	-0.45937	7.02719	6.56782
C^{+4}	-1.03407	7.60182	6.56775
N^{+5}	-1.52047	8.08819	6.56771
O^{+6}	-1.93701	8.50468	6.56767
F^{+7}	-2.30256	8.87021	6.56765
Ne^{+8}	-2.62828	9.19591	6.56763

Figure 5 shows (γ) and (γ) versus the parameter γ for He-like atomic system in HFR based on single zeta βTOs position space, while dotted points show the result of Farid et al. [35]. Equations 14 and 15, recover Equation 12-a as order $\gamma \to 1$. It is considered that $R_{\rho 1}$ and $T_{\rho 1}$ to the value of S_ρ due to undefined $R_{\rho 1}$ and $T_{\rho 1}$ at γ=1 due to the quantifies distribution of electron spreading of the system. Our results have good agreement with Ref. [35] (colored points). Furthermore, both R_ρ and T_ρ entropies decrease as increase in γ [28, 54–56]. Moreover, for γ>1, R_ρ is greater than T_ρ and possesses similar slopes, while for γ<1, T_ρ is higher and increases drastically than $R\rho$. The sign is changing as mentioned in Figure 5-a R_ρ for rises Z due to the reverse charge density of the Shannon entropy. For instance, at Z = 5, the sign of both $R_{\rho 1}$ and $R_{\rho 2}$ vary and our results agree with Farid et al. [33]. In Figure 5-b (γ) decreases for increasing Z. For $Z = 2$ and 3, S_ρ begins a huge positive value and reduces to zero gradually and changes the sign for various values of γ, whereas T_ρ has negative values at $Z \geq 5$.

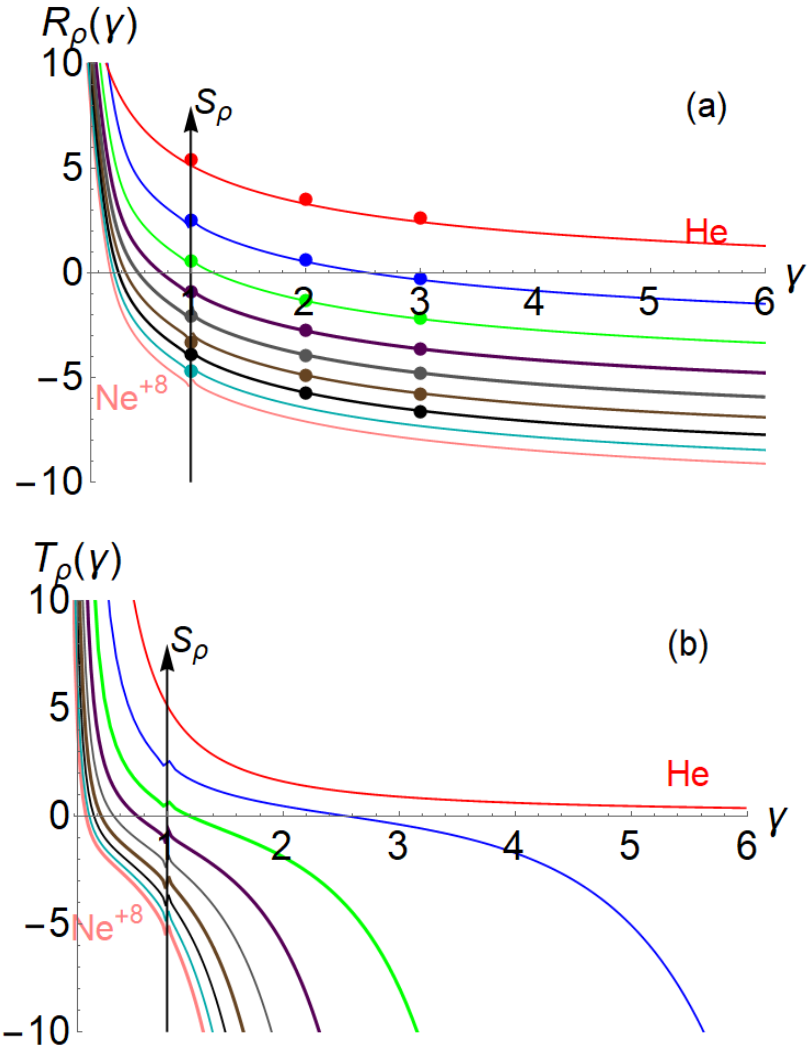

Figure 5. (a) R_ρ (γ) and, (b) T_ρ (γ) versus the parameter γ of $1s^2$ state for Helium-isoelectronic series in position space. Thepointed are the result of Farid et al. [35]

4- Conclusion

Electron density and information entropies have been studied within the HFR wave function obtained on single Zeta βTOs for ($2 \leq Z \leq 10$) atomic system atomic systems, where βTOs have the simple form of a linear combination of $STOs$ [40, 42]. The positions of maxima in radial electron probability density in position (momentum) space shift to smaller (larger) locations with increasing Z. The distribution of Shannon's entropy led to a significant effect on the distribution of the electron propagation in the system. The system of Shannon's entropy delocalization decreased with increasing Z. We have noticed the variation of S_ρ and S_Π for ($2 \leq Z \leq 10$) atomic systems, which deal with the interactions of the atom's nucleus and valence regions and thereby include a spatial understanding of the variation. In the limit $\gamma \to 1$, both R and T entropies tend to S_ρ. We have shown how the R, and T entropies decrease with increasing Z, whereas γ delocalizes as it reaches the ionization limit. Furthermore, since information entropies remain a subject of enormous research, our next suggestion is to propose information entropies for the ground and excited states of some atomic systems using correlated wave functions.

5- Declarations

5-1- Data Availability Statement

The data presented in this study are available on request from the corresponding author.

5-2- Funding

This work was supported by the College of Science, University of Al-Qadisiyah, Iraq.

5-3- Conflicts of Interest

The author declares that there is no conflict of interest regarding the publication of this manuscript. In addition, the ethical issues, including plagiarism, informed consent, misconduct, data fabrication and/or falsification, double publication and/or submission, and redundancies have been completely observed by the author.

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