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Shannon, Rényi, Tsallis Entropies and Onicescu Information Energy for Low-Lying Singly Excited States of Helium

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Abstract: Knowledge of the electronic structures of atomic and molecular systems deepens our understanding of the desired system. In particular, several information-theoretic quantities, such as Shannon entropy, have been applied to quantify the extent of electron delocalization for the ground state of various systems. To explore excited states, we calculated Shannon entropy and two of its one-parameter generalizations, Rényi entropy of order α and Tsallis entropy of order α , and Onicescu Information Energy of order α for four low-lying singly excited states ($1s2s\ ^1S^e$, $1s2s\ ^3S^e$, $1s3s\ ^1S^e$, and $1s3s\ ^3S^e$ states) of helium. This paper compares the behavior of these three quantities of order 0.5 to 9 for the ground and four excited states. We found that, generally, a higher excited state had a *larger* Rényi entropy, *larger* Tsallis entropy, and *smaller* Onicescu information energy. However, this trend was not definite and the singlet–triplet reversal occurred for Rényi entropy, Tsallis entropy and Onicescu information energy at a certain range of order α .

Keywords: Shannon entropy; Rényi entropy; Tsallis entropy; Onicescu information energy; singly excited states; helium; Hylleraas wave functions; singlet–triplet reversal

1. Introduction

The electronic structure, a unique feature of an atomic or molecular system, is fundamental for further understanding of other properties. To characterize an electronic structure, one critical aspect is whether the electron distribution is localized or delocalized [1,2]. Originated from the information theory and later extended to the position space, the *information-theoretic (IT) quantities* provide a possible quantitative account of the extent of electron localization. For instance, the more delocalized is the electron distribution, the larger is the Shannon entropy (S) [3–14]. Moreover, Rényi entropy of order α (R_α) [15–17] and Tsallis entropy of order α (T_α) [18–21] are the one-parameter generalizations of Shannon entropy and offer extended descriptions. In addition, Onicescu Information Energy of order α (E_α^O) [22,23] is related to the frequency moment of the electron density [24–26]. These IT quantities have been applied to various atomic and molecular systems [4–14,27–80] and potentials [81–91]. Further background details of these IT quantities were summarized by Ilić and Stanković [92] and by us [80].

However, a large part of the reports focus on the ground state, to the best of our knowledge. Even though some results for Rydberg states [10,40,46,62–64,81] are available, behaviors of these IT quantities for excited states remain to be explored. In particular, for the helium atom, Shannon entropy generally increases for higher excited states [10–12] but several exceptions are also found [10]. To examine the trend in IT quantities for increasing excitations, we calculated Shannon, Rényi, and Tsallis entropies and Onicescu Information Energy for four low-lying singly excited states ($1s2s\ ^1S^e$, $1s2s\ ^3S^e$, $1s3s\ ^1S^e$, and $1s3s\ ^3S^e$ states) of helium, subsequent to our previous benchmark report for the

ground state helium [80]. This paper compares the behavior of these quantities of order 0.5 to 9 for the ground and four excited states of helium.

2. Theoretical Methods

2.1. Determination of Ground and Singly Excited States of Helium via Hylleraas Wave Functions

The non-relativistic Hamiltonian of helium atom (in atomic units) is

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}},$$

where subscripts 1 and 2 are indexes of electrons, and r_{12} is the distance between the two electrons. Featuring the explicit r_{12} term, Hylleraas wave functions [93–95] take the electron correlation into account [96,97] and are written as

$$\psi_{mnk}(r_1, r_2, r_{12}) = \sum_{mnk} C_{mnk} (e^{-\beta_1 r_1} e^{-\beta_2 r_2} r_1^m r_2^n r_{12}^k + e^{-\beta_1 r_2} e^{-\beta_2 r_1} r_2^m r_1^n r_{12}^k)$$

for singlet states, and

$$\psi_{mnk}(r_1, r_2, r_{12}) = \sum_{mnk} C_{mnk} (e^{-\beta_1 r_1} e^{-\beta_2 r_2} r_1^m r_2^n r_{12}^k - e^{-\beta_1 r_2} e^{-\beta_2 r_1} r_2^m r_1^n r_{12}^k)$$

for triplet states. m, n, k , and ω are zero or positive integers and $m + n + k \leq \omega$ so ω determines the size of basis set. Besides, β_1 and β_2 are variational parameters. For singlet states with arbitrary β_1 and β_2 , and also for triplet states with $\beta_1 \neq \beta_2$, $m \geq n$ and ω starts from zero. On the other hand, for triplet states with $\beta_1 = \beta_2$, $m > n$ and ω counts from one. The restrictions above are summarized in Table 1.

Table 1. Restrictions on m, n and ω .

Spin Multiplicity Of The State	Relation between β_1 and β_2	Restriction on m and n	ω Starts from
singlet	$\beta_1 \neq \beta_2$		
singlet	$\beta_1 = \beta_2$	$m \geq n$	$\omega \geq 0$
triplet	$\beta_1 \neq \beta_2$		
triplet	$\beta_1 = \beta_2$	$m > n$	$\omega \geq 1$

2.2. Definitions for Electron Density

In the position space, Shannon, Rényi, and Tsallis entropies and Onicescu informational energy are defined in terms of the electron density. Nonetheless, different definitions of electron density exist in the literature and are described as follows. For a N -electron wave function $\Psi(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N)$, the *spinless one-electron density* [98], or *N -normalized one-electron density*, $\rho(\vec{r})$ is defined as

$$\rho(\vec{r}_1) \equiv N \int |\Psi(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N)|^2 ds_1 d\vec{x}_2 \dots d\vec{x}_N,$$

where $\vec{x}_i$ is the spin s_i and space $\vec{r}_i = (r_i, \theta_i, \phi_i)$ coordinates of the i th electron. Integration of this electron density equals to the number of electrons N in the system as

$$\int \rho(\vec{r}) d\vec{r} = N.$$

On the other hand, the *one-normalized one-electron density* $\sigma(\vec{r})$ is defined by dividing $\rho(\vec{r})$ by N as [99]

$$\sigma(\vec{r}) \equiv \frac{\rho(\vec{r})}{N}.$$

Therefore, in contrast to the former choice of normalizing the electron density $\rho(\vec{r})$ to N , $\sigma(\vec{r})$ is normalized to one as

$$\int \sigma(\vec{r}) d\vec{r} = 1.$$

This $\sigma(\vec{r})$ is also called *shape factor* [99,100], *shape function* [99,101], *unit-normalized density* [27], *1-normalized density* [29], or *density per particle* [102,103]. In this work, we computed the radial part of one-normalized one-electron density $\sigma(r_1)$ according to Calais and Lowdin as [104]

$$\begin{aligned} \sigma(r_1) &\equiv \frac{\rho(r_1)}{N} = \int |\psi(r_1, r_2, r_{12})|^2 d\vec{r}_2 \\ &= \frac{2\pi}{r_1} \int_0^\infty r_2 dr_2 \int_{|r_1-r_2|}^{r_1+r_2} r_{12} dr_{12} |\psi(r_1, r_2, r_{12})|^2. \end{aligned}$$

2.3. Information-Theoretic Quantities in the Position Space

In this work, we examined four information-theoretic quantities, including Shannon entropy (S), Rényi entropy of order α (R_α), Tsallis entropy of order α (T_α), and Onicescu informational energy of order α (E_α^O). These quantities originated from probability and information theory, and were later extended to the position space by taking the electron density as the argument. Further background details of these IT quantities are summarized in our previous work [80]. The information-theoretic quantities for one-normalized one-electron density $\sigma(r)$ are defined as

$$\begin{aligned} S[\sigma(r)] &\equiv - \int_0^\infty \sigma(r) \ln \sigma(r) 4\pi r^2 dr, \\ R_\alpha[\sigma(r)] &\equiv \frac{1}{1-\alpha} \ln \left[\int_0^\infty \sigma(r)^\alpha 4\pi r^2 dr \right], \\ T_\alpha[\sigma(r)] &\equiv \frac{1}{\alpha-1} \left[1 - \int_0^\infty \sigma(r)^\alpha 4\pi r^2 dr \right], \\ E_\alpha^O[\sigma(r)] &\equiv \frac{1}{\alpha-1} \int_0^\infty \sigma(r)^\alpha 4\pi r^2 dr. \end{aligned}$$

The integrals were solved by 600-point Gauss-Laguerre quadrature.

Although not calculated in this work, the information-theoretic quantities for N -normalized one-electron density $\rho(r)$ are defined similarly as

$$\begin{aligned} S[\rho(r)] &\equiv - \int_0^\infty \rho(r) \ln \rho(r) 4\pi r^2 dr, \\ R_\alpha[\rho(r)] &\equiv \frac{1}{1-\alpha} \ln \left[\int_0^\infty \rho(r)^\alpha 4\pi r^2 dr \right], \\ T_\alpha[\rho(r)] &\equiv \frac{1}{\alpha-1} \left[1 - \int_0^\infty \rho(r)^\alpha 4\pi r^2 dr \right], \\ E_\alpha^O[\rho(r)] &\equiv \frac{1}{\alpha-1} \int_0^\infty \rho(r)^\alpha 4\pi r^2 dr, \end{aligned}$$

Formulas for conversion between IT quantities using the two different densities are [27,29,32,55–57,59,72]

$$\begin{aligned} S[\rho(r)] &= S[\sigma(r)]N - N \ln N, \\ R_\alpha[\rho(r)] &= R_\alpha[\sigma(r)] + \frac{\alpha}{1-\alpha} \ln N, \\ T_\alpha[\rho(r)] &= T_\alpha[\sigma(r)]N^\alpha + \frac{1-N^\alpha}{\alpha-1}, \\ E_\alpha^O[\rho(r)] &= E_\alpha^O[\sigma(r)]N^\alpha. \end{aligned}$$

3. Results and Discussion

All values are in atomic units. We first examined the accuracy of calculated energy to confirm the quality of wave functions used for calculating other quantities. Moreover, the self consistency of our information-theoretic quantities were examined. Then, we compared and analyzed the behavior of the IT quantities for the ground and singly excited states.

3.1. Accuracy of Presented Energy and Information-Theoretic Quantities

3.1.1. Energy E

In our previous benchmark work for the ground state helium [80], we let $\beta_1 = \beta_2$ and changed only one parameter. In contrast, here for singly excited states, we varied β_1 and β_2 independently (Table 2) with size of basis set $\omega = 15$ (444 terms). Our energies satisfactorily agree with other high precision results [105] (Table 3), demonstrating the reliability of our calculations.

Table 2. Variational parameters β_1 and β_2 for the ground and low-lying singly excited states of helium with size of basis set $\omega = 15$.

State	β_1	β_2	State	β_1	β_2
1s1s $^1S^e$	2.00	2.00			
1s2s $^1S^e$	1.19	2.80	1s2s $^3S^e$	2.09	0.55
1s3s $^1S^e$	0.74	1.94	1s3s $^3S^e$	0.78	1.90

Table 3. Energy E and Shannon entropy S for the ground and low-lying singly excited states of helium with size of basis set $\omega = 15$.

State	E	S
1s² $^1S^e$	−2.903 724 371	2.705 102 85
Drake [105]	−2.903 724 377 034 119 5	
Lin and Ho [52]	−2.903 724 376 8	2.705 102 8
Ou and Ho [11]	−2.903 724 371	2.705 102 85
Restrepo Cuartas and Sanz-Vicario [10]	−2.903 605	2.705
1s2s $^1S^e$	−2.145 974 042	5.491 968 78
Drake [105]	−2.145 974 046 054 419 (6)	
Lin and Ho [106]	−2.145 974 042	
Ou and Ho [11]	−2.145 974 012	5.491 968 37
Katriel et al. [107]	−2.145 974 0	
Restrepo Cuartas and Sanz-Vicario [10]	−2.145 967	5.492
1s2s $^3S^e$	−2.175 229 377	5.235 978 14
Drake [105]	−2.175 229 378 236 791 30	
Lin and Ho [106]	−2.175 229 378 22	
Katriel et al. [107]	−2.175 229 4	
Restrepo Cuartas and Sanz-Vicario [10]	−2.175 229	5.236
1s3s $^1S^e$	−2.061 271 958	6.769 321 78
Drake [105]	−2.061 271 989 740 911 (5)	
Lin and Ho [106]	−2.061 271 96	
Restrepo Cuartas and Sanz-Vicario [10]	−2.061 270	6.769
1s3s $^3S^e$	−2.068 689 066	6.605 067 28
Drake [105]	−2.068 689 067 472 457 19	
Lin and Ho [106]	−2.068 689 06	
Restrepo Cuartas and Sanz-Vicario [10]	−2.068 689	6.605

3.1.2. Shannon Entropy S , Rényi Entropy R_α , Tsallis Entropy T_α and Onicescu Information Energy E_α^O

Our Shannon entropy well agreed with the literature [10,11,52,80] (Table 3). Moreover, we tested the self consistency by seeing if our values satisfy the analytic relations between them as follows. Let us take the $1s2s\ ^1S^e$ state for example (Figures 1 and 2). First, by definition, both Rényi entropy R_α and Tsallis entropy T_α recover Shannon entropy when the order α goes to one as

$$\begin{aligned}\lim_{\alpha \rightarrow 1} R_\alpha &= S, \\ \lim_{\alpha \rightarrow 1} T_\alpha &= S.\end{aligned}\quad (1)$$

Our numerical values obey this requirement because the curves of Rényi entropy and Tsallis entropy intersect each other at the value of Shannon entropy when order goes to one (Figure 1).

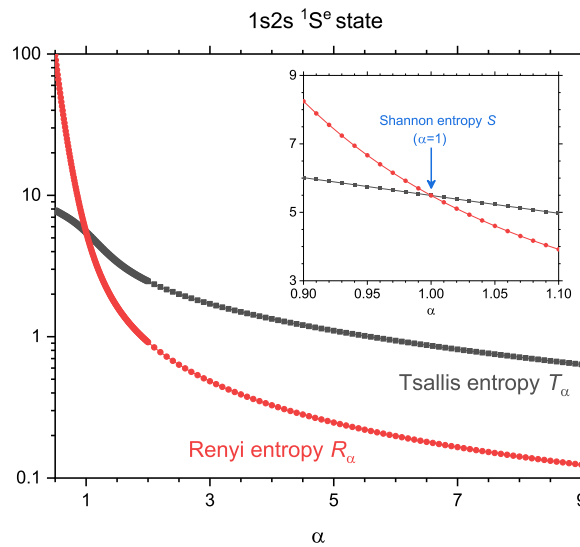


Figure 1. Rényi entropy R_α and Tsallis entropy T_α of order 0.5 to 9 of $1s2s\ ^1S^e$ state. Both recover the value of Shannon entropy as order α approaches one. Selected values are in Tables 4 and 5 and full data are in Tables S1 and S2.

Second, the sum of Tsallis entropy T_α and Onicescu informational energy E_α^O equals to $1/(\alpha - 1)$ as

$$T_\alpha + E_\alpha^O = \frac{1}{\alpha - 1} \quad (2)$$

This phenomenon is best seen in Figure 2. When the order α decreases toward 0.5, T_α increases, E_α^O decreases, and their sum $1/(\alpha - 1)$ tends to -2 . Furthermore, when the order is close α to one, Onicescu informational energy diverges, but the sum of Tsallis entropy and Onicescu informational energy still equals $1/(\alpha - 1)$.

Third, Rényi entropy R_α , Tsallis entropy T_α and Onicescu informational energy E_α^O are related by the following relations: [18,80]

$$\begin{aligned}R_\alpha &= \frac{\ln[1 + T_\alpha(1 - \alpha)]}{1 - \alpha}, \\ R_\alpha &= \frac{\ln[E_\alpha^O(\alpha - 1)]}{1 - \alpha}.\end{aligned}$$

Our numerical values fulfill these analytic relations between them.

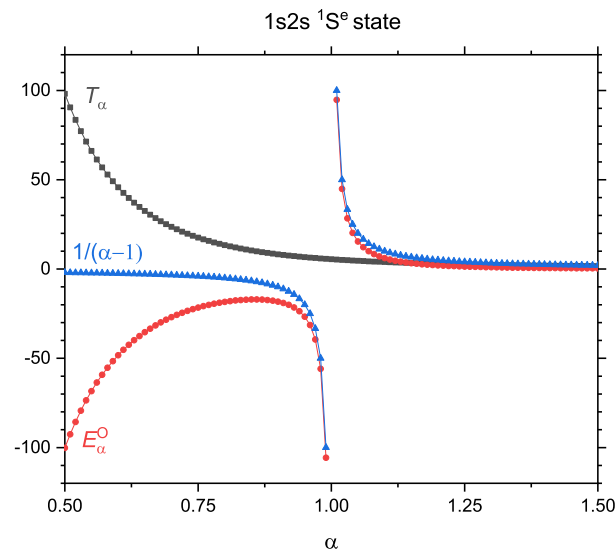


Figure 2. Tsallis entropy T_α and Onicescu informational energy E_α^O of order 0.50 to 1.50 of $1s2s\ ^1S^e$ state. The sum of Tsallis entropy and Onicescu Information Energy equals $1/(\alpha - 1)$. Selected values are in Tables 5 and 6 and full data are in Tables S2 and S3.

3.2. Comparison of Shannon Entropy S of the Ground and Four Singly Excited States

We first analyzed the behavior of Shannon entropy, from which Rényi entropy and Tsallis entropy were generalized. As shown in Table 3, the higher is the energy, the larger is the Shannon entropy [10–12]. However, although this trend was observed for the presented S -type states of helium, several exceptions have been reported if the states to be compared have different total orbital angular momentum L [10].

On the other hand, Shannon entropy reflects the extent of electron delocalization [10–12]. In particular, for a given configuration, the electron density of the triplet state is shift toward and more concentrated to the origin than that of the singlet (Figure 3). As a result, the triplet state has a lower Shannon entropy than the singlet. Restrepo Cuartas and Sanz-Vicario called this phenomenon the *Entropic Hund's first rule* [10].

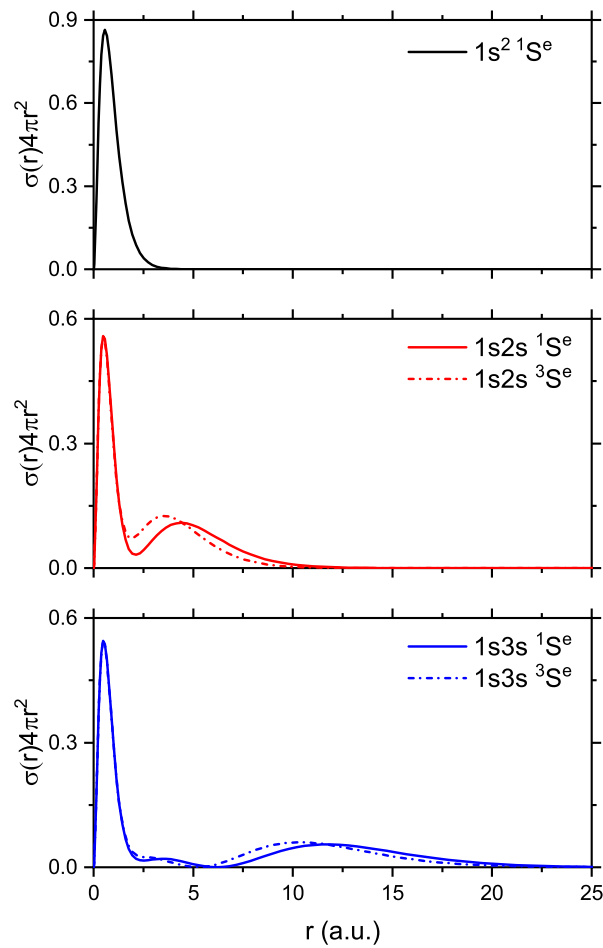


Figure 3. Radial probability density $\sigma(r)4\pi r^2$ for the ground and low-lying singly excited states of helium.

3.3. Comparison of Rényi Entropy R_α , Tsallis Entropy T_α and Onicescu Information Energy E_α^O of the Ground and Four Singly Excited States

Now, we move on to Rényi entropy R_α , Tsallis entropy T_α , and Onicescu Information Energy E_α^O . For simplicity, we consider the singlet states or the triplet states individually, and then compare the singlet with the triplet for a given configuration in the next subsection.

Within either the series of singlets ($1s^2\ ^1S^e$, $1s2s\ ^1S^e$ and $1s3s\ ^1S^e$ states) or the series of triplets ($1s2s\ ^3S^e$ and $1s3s\ ^3S^e$ states), higher excited states had *larger* Rényi entropy R_α (Figure 4a) and Tsallis entropy T_α (Figure 4b), and *smaller* Onicescu Information Energy (Figure 4c) throughout order α from 0.5 to 9. Furthermore, for a given IT quantity, the curves of different configurations gradually separate when the order α decreases toward 0.5. One possible explanation is that the electron distribution of higher excited states oscillated more (Figure 3), and this behavior may be highlighted at a certain range of order α .

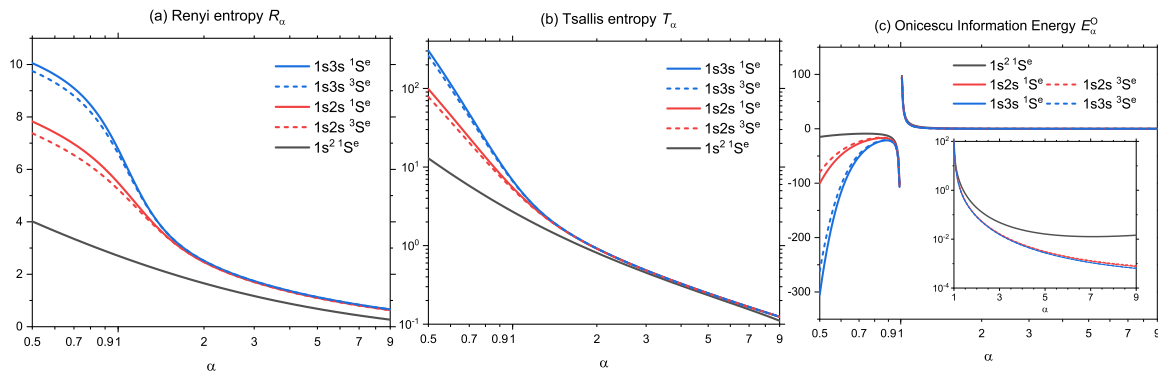


Figure 4. (a) Rényi entropy; (b) Tsallis entropy; and (c) Onicescu Information Energy of order 0.5 to 9 for the ground and low-lying singly excited states of helium with size of basis set $\omega = 15$. Selected values are in Tables 4–6. Full data are in Tables S1–S3.

3.4. Singlet–Triplet Reversal of Rényi entropy R_α , Tsallis entropy T_α and Onicescu Information Energy E_α^O

Here we compare the IT quantities of the singlet state with those of the corresponding triplet state. At first glance, for a given configuration, the singlet state generally had a *larger* Rényi entropy, *larger* Tsallis entropy and *smaller* Onicescu Information Energy than the triplet state (Figure 4). However, this ordering was not definite and may even be reversed. To be more specific, the difference between an IT quantity of the singlet state and that of the corresponding triplet state are in Figure 5a for the $1s2s$ and in Figure 5b for the $1s3s$ configuration. The singlet–triplet reversal occurred at $1.71 \leq \alpha \leq 2.2$ for the $1s2s$ and at $1.52 \leq \alpha \leq 2.8$ for the $1s3s$ configuration.

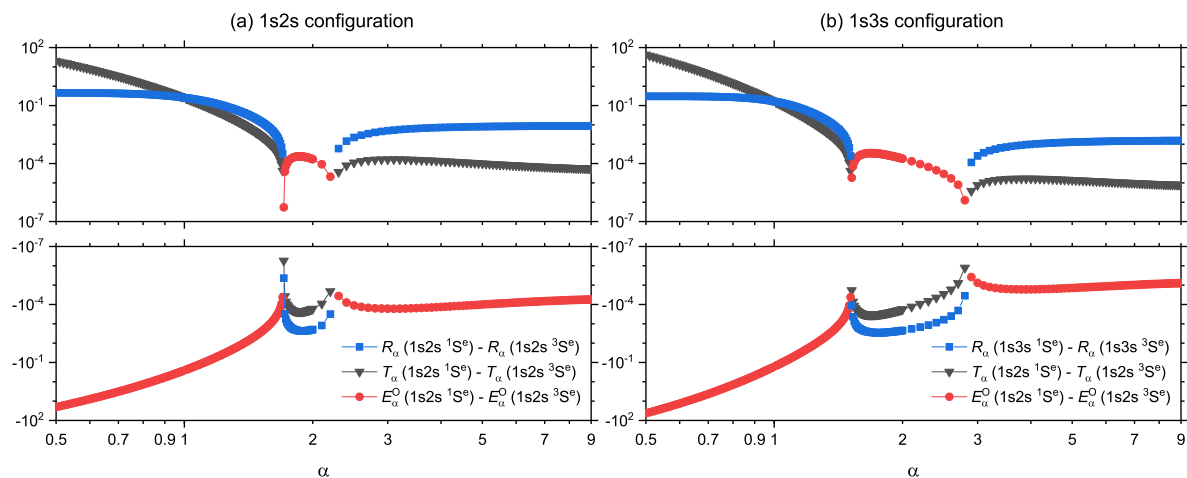


Figure 5. Singlet–triplet reversal of Rényi entropy R_α , Tsallis entropy T_α and Onicescu Information Energy E_α^O for: (a) $1s2s$; and (b) $1s3s$ configuration.

Moreover, the difference between Onicescu Information Energy of the singlet state and that of the triplet state has opposite sign to the difference for Tsallis entropy (Figure 5). This behavior can be readily verified by

$$\begin{aligned} E_\alpha^O(\text{singlet}) - E_\alpha^O(\text{triplet}) &= \left[\frac{1}{\alpha - 1} - T_\alpha(\text{singlet}) \right] - \left[\frac{1}{\alpha - 1} - T_\alpha(\text{triplet}) \right] \\ &= -[T_\alpha(\text{singlet}) - T_\alpha(\text{triplet})]. \end{aligned}$$

Selected values for Rényi, Tsallis entropy and Onicescu Information Energy for the low-lying singly excited states of helium are in Tables 4–6, respectively, and the full data are in Tables S1–S3.

Additionally, singlet–triplet reversal has also been reported for the interacting repulsive potential energy between two electrons in singly-excited states in quantum dots under certain confinement conditions [107,108], and in singly-excited states of helium-like ions under screened Coulomb interacting potentials with certain screening strengths and atomic numbers Z [109].

Table 4. Selected values for Rényi entropy of order α (R_α) for the low-lying singly excited states of helium with size of basis set $\omega = 15$. Values of R_1 are set to Shannon entropy. Full data are in Table S1.

α	1s2s		1s3s	
	$1S^e$	$3S^e$	$1S^e$	$3S^e$
0.5	7.827 360 64	7.375 384 22	$1.005\,154\,57 \times 10^1$	9.750 363 90
1	5.491 968 78	5.235 978 14	6.769 321 78	6.605 067 28
2	2.465 761 26	2.467 736 41	2.513 498 59	2.515 711 75
3	1.707 786 50	1.702 788 37	1.740 513 92	1.740 268 03
4	1.336 743 86	1.329 418 93	1.365 026 03	1.364 034 09
9	$6.372\,016\,65 \times 10^{-1}$	$6.284\,746\,43 \times 10^{-1}$	$6.602\,625\,52 \times 10^{-1}$	$6.587\,290\,39 \times 10^{-1}$

Table 5. Selected values for Tsallis entropy of order α (T_α) for low-lying singly excited states of helium with size of basis set $\omega = 15$. Values of T_1 are set to Shannon entropy. Full data are in Table S2.

α	1s2s		1s3s	
	$1S^e$	$3S^e$	$1S^e$	$3S^e$
0.5	$9.816\,586\,92 \times 10^1$	$7.790\,506\,90 \times 10^1$	$3.025\,758\,22 \times 10^2$	$2.599\,959\,72 \times 10^2$
1	5.491 968 78	5.235 978 14	6.769 321 78	6.605 067 28
2	$9.150\,558\,47 \times 10^{-1}$	$9.152\,234\,59 \times 10^{-1}$	$9.190\,155\,88 \times 10^{-1}$	$9.191\,946\,22 \times 10^{-1}$
3	$4.835\,712\,13 \times 10^{-1}$	$4.834\,061\,63 \times 10^{-1}$	$4.846\,121\,18 \times 10^{-1}$	$4.846\,045\,49 \times 10^{-1}$
4	$3.272\,902\,67 \times 10^{-1}$	$3.271\,560\,02 \times 10^{-1}$	$3.277\,818\,51 \times 10^{-1}$	$3.277\,653\,06 \times 10^{-1}$
9	$1.242\,360\,85 \times 10^{-1}$	$1.241\,808\,46 \times 10^{-1}$	$1.243\,647\,81 \times 10^{-1}$	$1.243\,569\,40 \times 10^{-1}$

Table 6. Selected values for Onicescu Information Energy of order α (E_α^O) for low-lying singly excited states of helium with size of basis set $\omega = 15$. E_α^O is undefined for $\alpha = 1$. Full data are in Table S3.

α	1s2s		1s3s	
	$1S^e$	$3S^e$	$1S^e$	$3S^e$
0.5	$-1.001\,658\,69 \times 10^2$	$-7.990\,506\,90 \times 10^1$	$-3.045\,758\,22 \times 10^2$	$-2.619\,959\,72 \times 10^2$
2	$8.494\,415\,29 \times 10^{-2}$	$8.477\,654\,09 \times 10^{-2}$	$8.098\,441\,11 \times 10^{-2}$	$8.080\,537\,79 \times 10^{-2}$
3	$1.642\,878\,69 \times 10^{-2}$	$1.659\,383\,68 \times 10^{-2}$	$1.538\,788\,10 \times 10^{-2}$	$1.539\,545\,02 \times 10^{-2}$
4	$6.043\,065\,38 \times 10^{-3}$	$6.177\,330\,33 \times 10^{-3}$	$5.551\,481\,84 \times 10^{-3}$	$5.568\,026\,65 \times 10^{-3}$
9	$7.639\,143\,64 \times 10^{-4}$	$8.191\,538\,09 \times 10^{-4}$	$6.352\,182\,23 \times 10^{-4}$	$6.430\,591\,45 \times 10^{-4}$

4. Conclusions

Generally, a higher excited state of helium had a *larger* Shannon entropy, *larger* Rényi entropy of order α , *larger* Tsallis entropy of order α , and *smaller* Onicescu information energy of order α . This behavior possibly reflects the more delocalized nature of electron distribution of higher excited states. However, for Rényi entropy, Tsallis entropy and Onicescu information energy, this trend was not definite and singlet–triplet reversal occurred at a certain range of order α . In the future, the knowledge of bounds and asymptotic analysis of these quantities may provide additional understanding of this behavior [110–116].

On the other hand, these IT quantities not only reflect the extent of electron delocalization, as discussed in this article, but also have numerous applications. For instance, Rényi entropy has been widely used to examine quantum entanglement [117–123]. Furthermore, Tsallis statistics is relevant to certain systems of ultracold atoms [124–127]. Moreover, these IT quantities are applied to investigate electron correlation [30,31,33,39,72,128–136] and various molecular properties as

well [28,36,45,48,49,59–61,72,73]. Calculated with the highly correlated Hylleraas wave functions, the results in this work then serve as a useful and reliable reference for the various applications mentioned above.

As for a theoretical application, our present calculations would also play a role to test the Collins Conjecture [137]—correlation energy (the difference between the exact energy and Hartree–Fock energy) is directly proportional to entropy—when one could extend the calculations to other helium-like ions. Thus, such a conjecture was tested by Dehesa and coworkers [138,139] to be valid for von Neumann entropy in helium iso-electronic sequence. It would be of interest to test the Collins Conjecture for Shannon, Renyi, or Tsallis entropy to be valid for helium sequence using highly correlated wave functions.

Finally, it should be mentioned that, to the best of our knowledge, there is no formula relating entropy to the quantum number of any given excited state, in a manner similar to the formula relating quantum defect to the effective quantum number for such an excited state. Nevertheless, this is an interesting issue and it is worthwhile to explore further in future investigations.

Supplementary Materials: Full data for Rényi, Tsallis entropies and Onicescu Information Energy of order 0.5 to 9 for the ground and low-lying singly excited states of helium are in Table S1 to S3 and are available online at <https://www.mdpi.com/2218-2004/7/3/70/s1>.

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