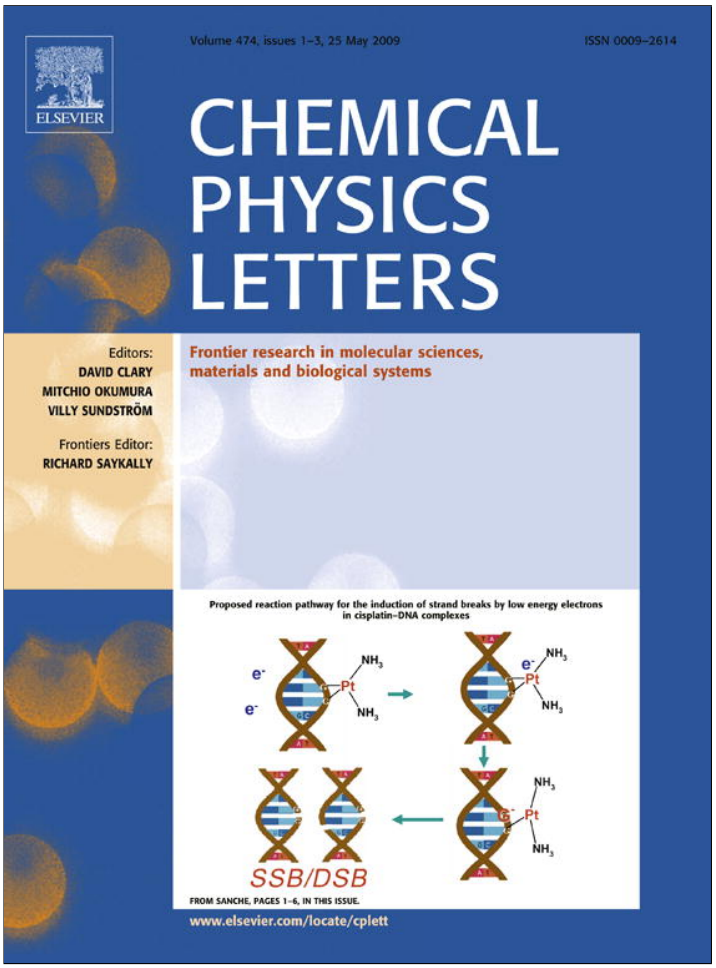

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Renyi complexities and information planes: Atomic structure in conjugated spaces

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ABSTRACT

Generalized Renyi complexity measures are defined and numerically analyzed for atomic one-particle densities in both conjugated spaces. These complexities provide, as particular cases, the previously known statistical and Fisher–Shannon complexities. The generalized complexities provide information on the atomic shell structure and shell-filling patterns, allowing to appropriately weight different regions of the electronic cloud.

1. Introduction

The study of complexity in physical, chemical, biological and social systems or processes is a topic of great contemporary research interest. A quantitative measure of complexity is useful to estimate the ability of systems for organization and it is also proposed as a general indicator of structure or correlation. Its controverted and difficult quantification has lead to a variety of definitions, e.g., algorithmic complexity [1,2], effective complexity [3], logical [4] and thermodynamical [5] depths, and computational [6] or statistical [7] complexities, but most of them share formal similarities with the others as well as with Bayes and information theories. Fundamental concepts such as entropy or information are frequently present in the proposals for characterizing complexity, but it is known that other ingredients capturing not only randomness are also necessary. In fact one would wish also to detect, for instance, clustering or pattern.

Recent proposals for a quantitative study of complexity try to formulate this magnitude as a product of two factors taking into account order/disequilibrium and disorder/uncertainty, respectively. These are the cases of the statistical complexity of López-Ruiz, Mancini, and Calbet (LMC) [7], the closely related two-parameter complexity of Shiner, Davison, and Landsberg (SDL) [8] or other product complexities [9].

The LMC complexity measure was originally defined as the product $D \cdot S$ of two important information-theoretic quantities: the disequilibrium D, which quantifies the departure of the probability distribution from uniformity [7,10] and the well known Shannon entropy, S, which is a universal measure of uncertainty or randomness [11]. On the other hand the SDL complexity is defined as the product of two factors, both constructed by using Shannon entropy, taking into account order and disorder, respectively, [8].

These product complexity measures, which satisfy the usual boundary conditions of minimum values in the extreme ordered and disordered limits, have been criticized and consequently modified leading to powerful estimators successfully checked in a wide variety of fields [12–15]. In particular the LMC complexity has been modified leading to the definition of 'shape complexity' $C(\mathrm{LMC}) = De^S$ [16–18] which satisfies several desirable properties of boundness [16,19] as well as invariance under scaling, translation and replication. The utility of this improved complexity has been shown in many fields [13,15,20,21] and also allows reliable detection of quasiperiodic and linear stochastics, and nonlinear dynamics [18].

Recently some other product complexities have been also studied. Such is the case of the so called Fisher–Shannon complexity $C(\mathrm{FS}) = I \cdot J = I \cdot (1/2\pi e)e^{2S/n}$ of n-dimensional distributions, which incorporates an important magnitude of local character: the Fisher information I [22,23]. This information measure quantifies the gradient content of the probability distribution and therefore explores deeply the internal changes it suffers. Numerical factors in the FS complexity are chosen to have the rigorous bound $C(\mathrm{FS}) \geqslant n$ [24].

The above LMC and FS complexity measures, their components and some other related magnitudes have been applied recently to the study of multielectron systems by means of their monoparticular electron densities in conjugated spaces [9,25–27].

The FS complexity has been applied only in very few fields, in spite of their success, including the pioneering work on analysis of signals [24], a study of electron correlation [28] and some other works studying atomic systems and ionization processes [29,30]. Very recently additional analytic works in the field of quantum mechanics have also used the FS complexity [31–34].

Some complexity studies in atoms were carried out, but most of them only for non-heavy systems (nuclear charge up to $Z = 54$ [35]) or only in the usual position space [36]. It has been very re-

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cently that studies on the electronic structural complexity of atomic systems, taking into account momentum space, were reported [9,37]. It has been shown that it is not sufficient to study the above measures only in the usual position space, but also in the complementary momentum space, in order to have a complete description of the information theoretic internal structure and the behavior of physical processes suffered by these systems. Some other new proposals of product-type complexity measures (e.g., Cramer–Rao complexity) have been also constructed and computed for multielectronic systems [9].

In this work we study a generalization of these product-like complexities by replacing the Shannon entropy functional by a more general and powerful magnitude as the Renyi entropy. Therefore we deal with a one-parameter (to be denoted by α) generalized complexity which weights different regions of the position or momentum spaces according to the value of α. The LMC and FS complexities are particular cases of these so-called Renyi complexities.

In concrete the so-called 'Shape Renyi complexity' (SR), characterized as a difference between the α-order Renyi entropy and the second-order one (expressed in terms of the disequilibrium, D), has been extended to continuous systems [14], theoretically studied, and tested for the binary symmetric channel (BSC) and the logistic map [20]. A more extended family of generalized complexity measures has been proposed, and rigorous bounds, geometrical properties and several applications have been also studied [38].

Moreover, the 'Fisher–Renyi complexity' (FR) is defined by simply replacing the Shannon entropy by the Renyi entropy in the expression of the Fisher–Shannon complexity. Some rigorous properties for this entropic product, also called Fisher–Renyi product, and similar ones have been recently obtained [39].

Previous applications of both the SR and FR complexities within the framework of the present manuscript, i.e. their interpretation according to the shell structure of atomic systems, are very scarce in the literature. To the best of our knowledge, in fact, this is the first time in which the SR complexity is considered and analyzed for atoms. The same also occurs with the FR complexity, apart from recently derived results [39], mainly concerning uncertainty-like relationships but not the atomic structure and the shell-filling process.

In this work we use both generalized Renyi complexities, SR and FR, to study the behavior of simple quantum-mechanical systems, but strongly organized and hierarchical, such as the neutral atoms throughout the whole Periodic Table of elements. In Section 2 a complete numerical study of these complexities at the Hartree–Fock level is done for the atomic position and momentum one-particle densities, revealing the complementary and fundamental roles of both conjugated spaces. Complex patterns and localization–delocalization planes are also investigated within Section 3 in both spaces, and conclusions and main results are collected in the last section.

2. Fisher–Renyi and Shape Renyi complexities

The concept of Renyi complexity arises from the delocalization or entropy measure of identical name, widely used in the literature when affording many different problems within an information-theoretic framework [40]. The Renyi entropy plays a similar role to those of other density functionals as descriptors of the uncertainty on a distribution. Among them, very well-known ones are the Shannon [11] and the Tsallis [41] entropies. However, the complexity of a given system also provides information on its level of localization or order, by means of information measures such as, e.g., the disequilibrium or the Fisher information.

The Renyi entropy of order α for a distribution $\rho(\vec{r})$ defined over the three-dimensional space is defined as

$$R^{(\alpha)} \equiv \frac{1}{1-\alpha} \ln \omega_\alpha \tag{1}$$

where the quantity ω_α is the so-called 'α-order frequency moment' of $\rho(\vec{r})$, given by

$$\omega_\alpha \equiv \int \rho^\alpha(\vec{r}) d\vec{r}, \tag{2}$$

which have been also employed in diverse fields, specially remarkable being their meaning for some specific α values in the development of the Density Functional Theory [42] (e.g., Thomas–Fermi kinetic and exchange energies) as well as the own disequilibrium [7,10]. The normalization to unity of the distribution can be expressed as $\omega_1 = 1$.

The allowed range of values for the characteristic parameter α of the Renyi entropy is determined by the convergence conditions on the integral in Eq. (2), being imposed by the short- and long-range behaviors of the distribution $\rho(\vec{r})$. Apart from the necessary (but not sufficient) condition $\alpha > 0$ for the finiteness of $R^{(\alpha)}$, the particular value $\alpha = 1$ appears as a limiting case, because both the numerator and the denominator in Eq. (1) vanish, the limit giving rise to

$$R^{(1)} = S = -\int \rho(\vec{r}) \ln \rho(\vec{r}) d\vec{r}, \tag{3}$$

that is, the Renyi entropy of order 1 is the Shannon entropy S or, in other words, the Renyi entropy $R^{(\alpha)}$ represents an extension or generalization of the Shannon entropy.

The power α of the distribution in Eq. (2), where ω_α is defined, allows to enhance or diminish, by increasing or decreasing its value, the contribution of the integrand over different regions to the whole integral and, consequently, to the frequency moments and the Renyi entropy $R^{(\alpha)}$. Higher values of α make the function $\rho^\alpha(\vec{r})$ to concentrate around the local maxima of the distribution, while the lower values have the effect of smoothing that function over its whole domain. It is in that sense that the parameter α provide us with a powerful tool in order to get information on the structure of the distribution by means of the Renyi entropy.

A relevant particular case of the Renyi entropy and the frequency moments corresponds to $\alpha = 2$, from which arises the definition of 'disequilibrium' D as the second-order frequency moment ω_2, namely

$$D \equiv \int \rho^2(\vec{r}) d\vec{r}, \tag{4}$$

which is a well-known descriptor of the 'level of departure from uniformity' of the distribution [7,10]. According to its definition and that of $R^{(\alpha)}$ it is immediate to observe that $R^{(2)} = -\ln D$, establishing a link between the Renyi entropy and the disequilibrium.

All quantities defined in the present section, playing a relevant role within an information-theoretic context, posses a 'global character', in the sense that they are very little sensitive to strong changes on the distribution over a small-sized region. Such is not the case of another information functional, known as 'Fisher information' I, which constitutes a measure of the gradient content of the distribution, being much more sensitive to those strongly localized perturbations. It is defined as [22]

$$I \equiv \int \rho(\vec{r}) |\vec{\nabla} \ln \rho(\vec{r})|^2 d\vec{r}, \tag{5}$$

where the gradient operator significantly determines the contribution of the aforementioned variations of the distribution over its domain to the value of the Fisher information. This is the reason of

such a measure I being usually referred as a 'local' descriptor, according to its sensitivity to local characteristics of $\rho(\vec{r})$.

As described in Section 1, the main complexity measures are usually built up as the product of two factors, such being the case of the LMC and FS complexities. In both of them, the Shannon entropy S is employed as measure of information in one factor, the other factor (measure of order) being the disequilibrium D and the Fisher information I for the LMC and FS complexities, respectively. The first aim of this section is to define and analyze a generalized version of the aforementioned complexities, where the Shannon entropy contribution is replaced by the Renyi entropy $R^{(\alpha)}$, giving rise to generalized complexity measures which will be referred as 'Shape Renyi complexity' $\mathrm{SR}^{(\alpha)}$ and 'Fisher–Renyi complexity' $\mathrm{FR}^{(\alpha)}$, defined as

$$\mathrm{SR}^{(\alpha)} \equiv D \cdot \exp\{R^{(\alpha)}\}, \tag{6}$$

with the exponential Renyi entropy being also denoted as $L^{(\alpha)} \equiv \exp\{R^{(\alpha)}\}$, and

$$\mathrm{FR}^{(\alpha)} \equiv I \cdot J^{(\alpha)}, \tag{7}$$

where

$$J^{(\alpha)} = \frac{1}{2\pi e} \exp\left\{\frac{2}{3} R^{(\alpha)}\right\} \tag{8}$$

is the 'α-order power entropy' for the three-dimensional case.

Some comments are in order: (i) the particular cases $\mathrm{SR}^{(1)}$ and $\mathrm{FR}^{(1)}$ corresponding to $\alpha = 1$ provide, respectively, the expressions of the LMC and FS complexities, (ii) all relevant invariance properties of LMC and FS also remain for arbitrary $\alpha > 0$, (iii) the weighting effect of the parameter α over specific regions, as previously mentioned for the Renyi entropy, now translates into the associated complexities, and (iv) attending to its definition, the composing factors of the second-order Shape Renyi complexity are one the inverse of the other, and consequently $\mathrm{SR}^{(2)} = 1$.

Other Renyi products have been also considered in the literature, for which different properties such as, e.g., bounds and uncertainty-like relationships are known for very specific α ranges [39]. The analysis of those properties is not within the aims of the present job, in which a much wider interval for the α parameter is considered.

The next purpose is to analyze numerically the Shape Renyi and Fisher–Renyi complexities of the one-particle densities in position and momentum spaces, $\rho(\vec{r})$ and $\gamma(\vec{p})$, respectively, for neutral atoms throughout the Periodic Table, their nuclear charge ranging from $Z = 1$ to $Z = 103$. In doing so, the accurate near Hartree–Fock wavefunctions of Koga et al. [43] are employed. For atomic systems in the absence of external fields, as in the present case, it is sufficient to deal with the spherically averaged densities $\rho(r)$ and $\gamma(p)$.

The Shape Renyi complexity in position and momentum spaces, to be denoted by $\mathrm{SR}_r^{(\alpha)}$ and $\mathrm{SR}_p^{(\alpha)}$, respectively, are shown for these atomic systems in Fig. 1a (position) and b (momentum), for diverse values of the parameter α within the range $0.4 \leqslant \alpha \leqslant 3.6$, corresponding to the different curves displayed. It is worthy to point out that for atomic systems the exponential long-range behavior of the position space density [44] allows any non-negative value $\alpha > 0$, while the momentum space one as p^{-8} [45] imposes the constraint $\alpha > 3/8 = 0.375$.

A first look at Fig. 1 allows to observe relevant differences between the structural characteristics of the Shape Renyi complexity $\mathrm{SR}^{(\alpha)}$ after comparing the curves corresponding to both conjugated spaces. The position space measure $\mathrm{SR}_r^{(\alpha)}$ (Fig. 1a) displays a much richer structure when dealing with very low values of α, reaching a higher smoothness and monotonicity as α increases. In those cases where the presence of local extrema is more apparent, a detailed analysis of their location reveals that they correspond either to

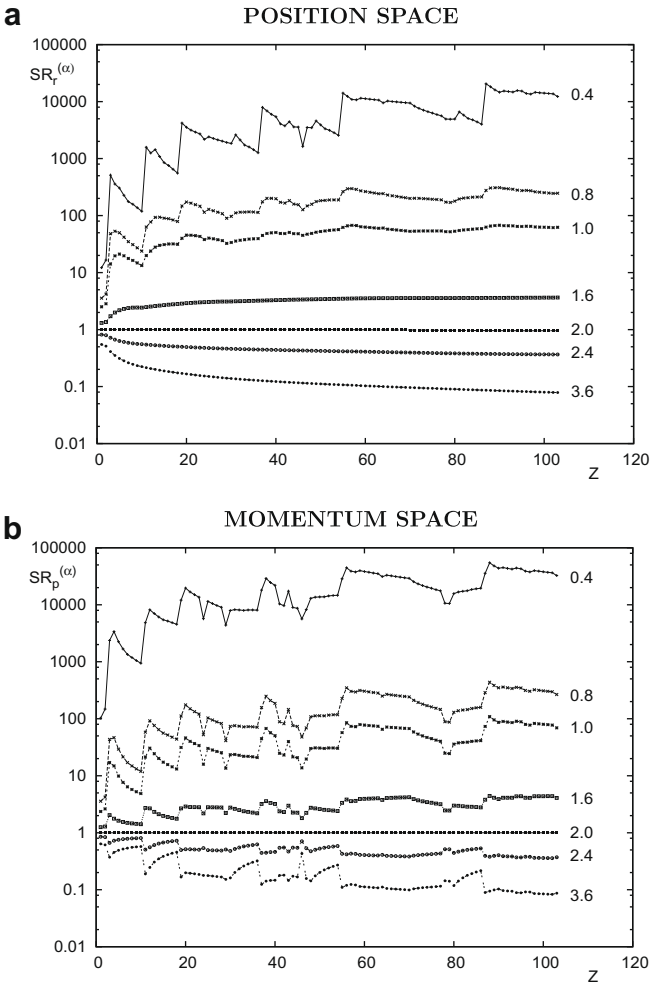

Fig. 1. Shape Renyi complexity $\mathrm{SR}^{(\alpha)}$ for $\alpha = 0.4, 0.8, 1.0, 1.6, 2.0, 2.4, 3.6$ in (a) position space and (b) momentum space. Atomic units (a.u.) are used.

closed shell systems or to atoms suffering the so called 'anomalous shell-filling'. These two characteristics depend on the occupation number of the outermost or the valence atomic subshell, where the aforementioned exponential behavior of $\rho(r)$ makes the density values to be very small as compared to those of the core region. Consequently, powering the density to a small α value enhances the contribution of the valence region, revealing the properties associated to the shell-filling process. Specially relevant is the strength for systems with 's' valence subshell as compared to other values of the angular momentum quantum number. It is additionally observed that changes of the $\mathrm{SR}^{(\alpha)}$ in both spaces when increasing the nuclear charge (i.e. between consecutive systems) become smaller as far as considering heavier atoms, being much apparent for light ones.

The same study in momentum space (Fig. 1b) provides similar conclusions in what concerns the location of extrema and its interpretation in terms of the shell structure. The main difference when comparing to the position space curves is that such a structure is displayed independently of the α value consider, being much more apparent again for lower α's. Nevertheless, even for high α values that structure can be also observed under a much smaller scale. Again the reason for finding this behavior can be understood having in mind that the valence region is populated by low speed electrons, represented in terms of the momentum density $\gamma(p)$ by its value around the origin (i.e. close to $p = 0$). The momentum density in that region reaches high enough values in order to provide

information on the valence electrons even without carrying out the enhancement operation by lowering the α parameter.

Similar comments to those arising from the analysis of the figure corresponding to the Shape Renyi complexity $SR^{(\alpha)}$ in both conjugated spaces remain also valid for the Fisher–Renyi complexity $FR^{(\alpha)}$ as observed in Fig. 2, at least in what concerns location of extrema and level of structure in each space. Fig. 2 is composed similarly as Fig. 1, i.e. position space (Fig. 2a) and momentum space (Fig. 2b). At this point it is worthy to remember the very different character of the factors involved as measures of order for each complexity, namely the disequilibrium and the Fisher information, respectively. In spite of such a difference, the complexities themselves display a very similar structure for all the α values here considered. Nevertheless, a detailed analysis reveals the aforementioned 'local sensitivity' of the Fisher–Renyi complexity $FR^{(\alpha)}$ as compared to the Shape Renyi one $SR^{(\alpha)}$ in the magnitude of their variations for closed shells and anomalous shell-filling systems, specially in the momentum space, much less visible in the position one.

It should be pointed out the role played by the Renyi complexities SR and FR as compared to the individual factors composing them. It is well known the monotonic and structureless behavior of, e.g., the disequilibrium D_r or the Fisher entropy I_r in position space [29], as also recently observed for the Renyi entropy $R_p^{(\alpha)}$ with $\alpha > 1$ [46].

The study of Figs. 1 and 2 reveals not only the interest of considering different values of the Renyi parameter α in order to obtain a more complete information on the density structure in different atomic regions from the Renyi-like complexities, but also the usefulness of dealing simultaneously with both position and momentum spaces.

3. Renyi information planes

Far beyond the Shape Renyi and Fisher–Renyi atomic complexities as descriptors of the shell-filling pattern and information content, it appears also relevant the study of the contribution to the whole complexity of each of its composing factors, in order to analyze the location of all atomic systems here considered in the corresponding order–disorder plane. In this way, systems belonging to similar complexity values can be also classified attending to their disequilibrium/order on one hand, and to their uncertainty/disorder on the other.

For illustration, the corresponding I–$J^{(\alpha)}$ and D–$L^{(\alpha)}$ planes are shown in Figs. 3 and 4, respectively, in the position space for the first case (i.e. I_r–$J_r^{(\alpha)}$ in Fig. 3) and in the momentum one for the other (i.e. D_p–$L_p^{(\alpha)}$ in Fig. 4). Similar conclusions are obtained for the other planes: for a given space, both planes look similar, the differences being mainly associated to the global and local character of the involved factors, as will be explained when discussing Figs. 3 and 4 in detail. Nevertheless, it should be remarked that momentum space planes appear more involved than the position ones. As mentioned in the previous section, the information content of the atomic systems is mainly governed by the nuclear region in position space and by the valence subshells in the momentum one. Adding electrons to the atomic systems is a process which follows rules (shell-filling pattern) not as simple as merely increasing the nuclear charge. Such a difference is also displayed in the corresponding information planes.

Fig. 3 displays the Fisher–Renyi plane in position space, for different values of the parameter α. The main two comments arising from the analysis of this figure are: (i) as observed in Section 2 for the position space complexities, the atomic shell structure is displayed, also in the information planes, for low α values, the curves being very smooth and almost monotonic for higher ones; the location of peaks corresponding to local extrema are associated to the characteristics of the atomic shell-filling, and (ii) all curves display a similar trend of large Fisher information and low power entropy for heavy atoms, which can be interpreted as a relevant increase of

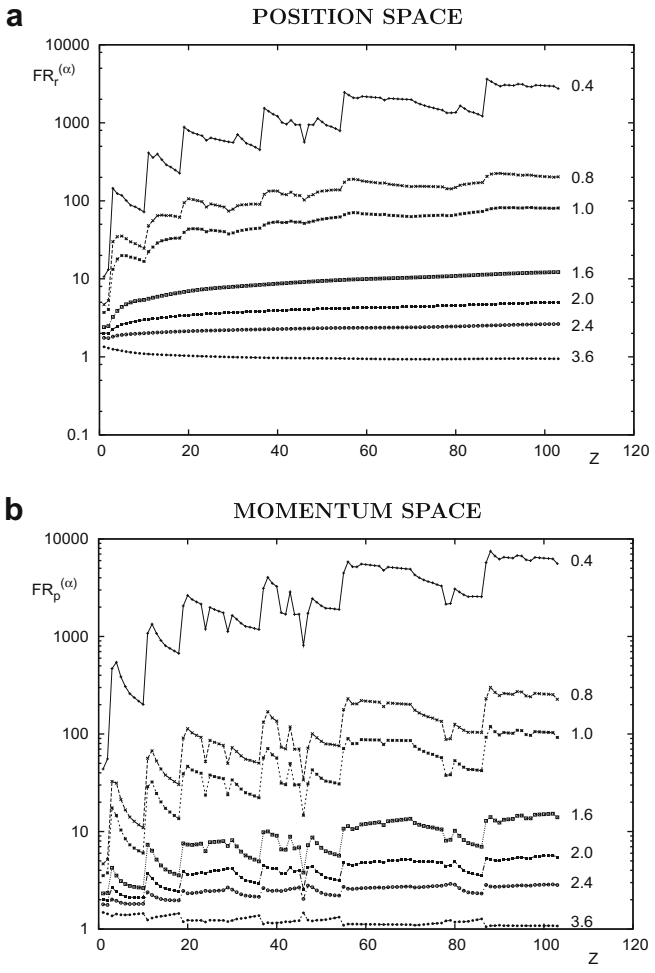

Fig. 2. Fisher–Renyi complexity $FR^{(\alpha)}$ for $\alpha = 0.4, 0.8, 1.0, 1.6, 2.0, 2.4, 3.6$ in (a) position space and (b) momentum space. Atomic units (a.u.) are used.

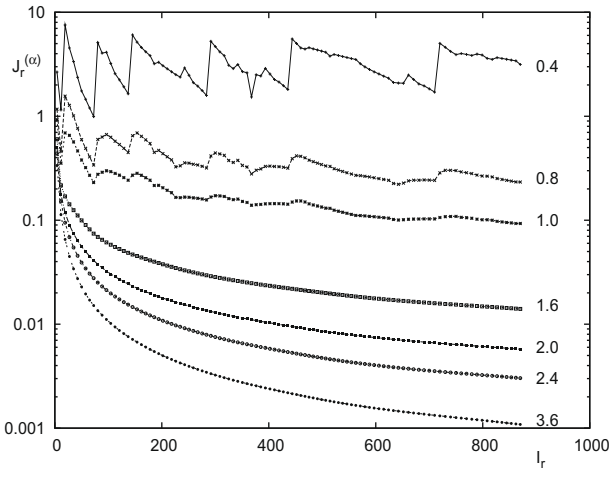

Fig. 3. Fisher–Renyi plane I–$J^{(\alpha)}$ in position space, for $\alpha = 0.4, 1.0, 2.0, 3.6$. Atomic units (a.u.) are used.

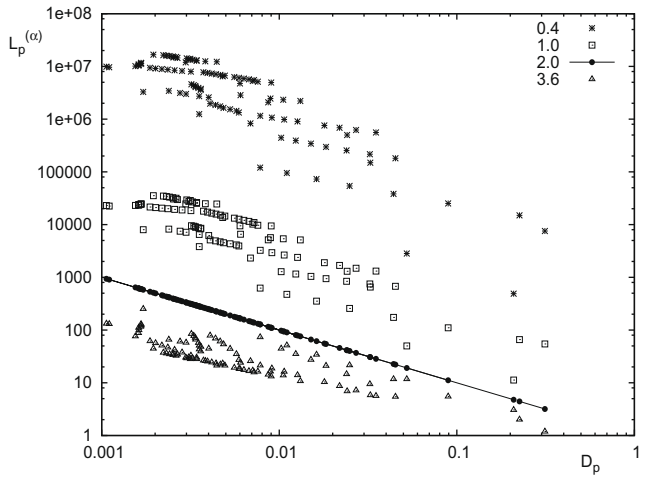

Fig. 4. Shape Renyi plane $D{-}L^{(\alpha)}$ in momentum space for $\alpha = 0.4, 0.8, 1.0, 1.6, 2.0, 2.4, 3.6$. Atomic units (a.u.) are used.

gradient at the origin as the electron cloud concentrates around the nuclear region when the nuclear charge increases, while in other regions the electron density spreads almost uniformly, increasing consequently the power entropy.

The aforementioned involvement in momentum space as a consequence of the shell-filling process is clearly observed in Fig. 4, where the location of the different atomic systems in the momentum $D{-}L^{(\alpha)}$ plane for a given value of the parameter α are displayed as a 'cloud', instead of a curve as in previous figures (apart from the trivial case $\alpha = 2$ with a constant $SR^{(\alpha)}$ product). Nevertheless, it is observed a general trend for each α value, in the sense that heavy systems concentrate around the upper-left region, corresponding to low disequilibrium and high exponential entropy (i.e. low order and high uncertainty). Additionally, the distance between consecutive systems becomes shorter as increasing their nuclear charge. In what concerns the dependence on α, it is observed that the clouds are ordered from above to below as increasing α, belonging to different bands, parallel to the unity product line.

A comparison between Figs. 3 and 4 perfectly shows the complementary character of the two conjugated spaces as well as that of the contributing individual factors to the whole complexity in both information planes. In this sense, it is worthy to remark that heavy systems are located, in the position space plane, in the lower right corner, corresponding to a high localization and a low entropy. Opposite trends, however, are observed in momentum space.

As in the complexity figures, it is also possible to distinguish the shell-filling patterns for low α in momentum space, more clearly for inner subshells (i.e. 1s, 2s, 2p). Nevertheless, the same can be also observed for additional subshells by employing an appropriate scale in the figure.

4. Conclusions

The Shape Renyi and Fisher–Renyi complexities generalize other ones previously employed for analyzing atomic densities, including them as particular cases. The characteristic parameter of the Renyi complexities allows to modify the relative weight of the distribution within specific regions of physical interest. The numerical study carried out in the present work provides relevant information on the atomic shell structure as well as the uncertainty and disequilibrium patterns in both conjugated spaces for neutral atoms throughout the whole periodic table. The complementary role played by the involved information measures, of very different character, appears very relevant especially when dealing simultaneously with the position and momentum distributions. Each one behaves in a characteristic fashion according to the nuclear charge of the involved systems, as well as to their valence subshells and the groups they belong to.

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