A generalized relative complexity: Application to atomic one-particle densities

P.A. Bouvrie [a,c], J.C. Angulo [a,c,*], J. Antolín [b,c]

[a] Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada, 18071 Granada, Spain
[b] Departamento de Física Aplicada, EINA, Universidad de Zaragoza, 50018 Zaragoza, Spain
[c] Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, 18071 Granada, Spain

ARTICLE INFO

ABSTRACT

The search of an appropriate measure of relative complexity among density functions is afforded. In doing so, the main properties required for complexity functionals of a given distribution, as well as those for discrimination measures among two or more distributions are considered. A proposal for a generalized relative complexity is provided, enclosing a pioneering definition as a limiting case. A theoretical analysis of the generalized measure for arbitrary distributions is carried out. The applications regard the electron charge densities of neutral atoms, and the results are interpreted on the basis of the main physical properties of the systems considered.

© 2012 Elsevier B.V. All rights reserved.

1. Introduction

Information-theoretical tools have been increasingly applied in several disciplines ranging from chemistry, physics, genetics, neural networks, computer science, image recognition to linguistics or social sciences [1–4]. Quantum Information Theory [5] and the study of entanglement [6,7] are recent examples of the versatility of information theory techniques to be applied in new fields of scientific or technological interest. In particular there has been a tremendous interest in the literature to apply information theory to quantum mechanical systems [8,9], to study the electronic structure of atoms and molecules [10–12] or even to explore some chemical processes such as ionization or chemical reactions [13,14].

The concepts of uncertainty, randomness, correlation, organization, information, disorder or delocalization are basic ingredients in the study of relevant properties for many probability distributions appearing as descriptors of chemical or physical systems or processes. These concepts concerning individual distributions are quantified by means of closely related and well known density functionals, such as Shannon entropy [15], Fisher Information [16] or disequilibrium [17]. Other relevant magnitudes, dependent on two (or more) different densities, have been also defined, studied and applied to detect similarity, clustering or discrepancy, as comparative measures among them [18,19].

Another relevant concept within Information Theory is complexity [20–23], strongly related, in some cases, to the aforementioned magnitudes. Indeed some of the recent definitions of complexity consist of the product of two factors measuring, respectively, order and disorder on the given system or process, or equivalently localization and delocalization [24]. It is important to note here that there is not a unique and universal definition of complexity and therefore many mathematical quantifications exist to explore pattern, structure or uncertainty as complexity ingredients or indicators. Complexity is used in very different fields including, for instance, molecular and DNA (deoxyribonucleic acid) analyses, dynamical systems, time series, spatial patterns or analysis of multielectronic systems, which is the focus of interest in this work [22,25,26].

The product complexity measures were criticized and consequently modified, leading to powerful estimators applied in a wide variety of fields [25,27,28]. Following the pioneering product measure of López-Ruiz, Mancini and Calbet (LMC complexity) [24] some other related and generalized complexity measures were defined and successfully applied [25,29–31].

A thorough discussion on the meaning and properties of atomic and molecular complexities can be found in Refs. [26,31–33] and Chapter 6 of Ref. [20]. In the atomic case, it is clearly established the connection between the complexity values of the electron densities and physically relevant properties. It is worthy to remark the interpretation in terms of the organization of electrons into shells and subshells, for both neutral and ionized systems. Additionally, the complexity analysis of atomic ionization processes provides further connections with the value of the ionization potential, as well as with the quantum numbers of the electron(s) ejected or added. In all these studies, a more complete information is achieved when dealing simultaneously with the one-particle densities in both conjugate spaces, namely position and momentum.

Complementary with the just mentioned numerical studies, rigorous bounds on the complexity in terms of physical observables

* Corresponding author at: Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada, 18071 Granada, Spain.
   E-mail address: angulo@ugr.es (J.C. Angulo).

are also known [31]. Specially relevant are those expressed in terms of radial expectation values of both the position and momentum electron densities. Some of these observables are related to relevant physical quantities, such as e.g. the kinetic energy and its relativistic correction, the electron-nucleus attraction energy or the diamagnetic susceptibility, among others.

Very recently new statistical relative complexities have been defined [34,35], and the pioneering LMC-like one has been applied to atomic densities [34]. This is an intrinsic measure that compares more efficiently the complexity of two electronic distributions, rather than merely the difference of their absolute complexities. Important properties have been also shown for this relative complexity, but the numerical tests are limited to some selected cases.

In this work we define a two-parameter generalized relative complexity, which contains the above mentioned relative complexity in Ref. [34] as a particular case and fulfills the most important complexity properties. Furthermore this relative complexity is extended and applied to more than two densities, their relative weights can be modulated if necessary, and also allows, by using appropriate values of its parameters, to enhance more or less different regions of the densities according to specific properties of the distributions. Some numerical difficulties of the original relative complexity are also marked.

The Letter is organized as follows. In the Section 2 the generalized relative complexity is defined and its main properties are shown. In Section 3 numerical tests have been done for atomic electron densities. Conclusions and open questions are presented in Section 4.

2. Relative complexity: a two-folded generalization

The recently introduced [34] LMC-like relative complexity of system A with respect to system B,

$$C(A,B) = D(A,B) \cdot H(A,B) \tag{1}$$

is based on the definition of the pioneering LMC complexity for a unique system [24], namely

$$C(A) = D(A) \cdot H(A). \tag{2}$$

For the most general definition of a product-like complexity, the factor $H(A)$ is a measure of disorder or delocalization of the representative density function $\rho_A(\vec{r})$ for system A, while the factor $D(A)$ constitutes a measure of its 'disequilibrium', that is, of its departure from equilibrium. In the case of the LMC complexity [24], the delocalization factor is defined in terms of the Shannon entropy [15] $S(A) = -\int \rho_A \ln \rho_A d\vec{r}$ as

$$H(A) = \exp\{S(A)\}, \tag{3}$$

a quantity referred as 'exponential entropy'. On the other hand, the disequilibrium is given by [17]

$$D(A) = \int \rho_A^2 d\vec{r}. \tag{4}$$

Normalized to unity distributions will be considered throughout.

The complexity $C(A)$ given by Eq. (2) constitutes a measure of pattern, structure and correlation in systems and processes. Its relative version $C(A,B)$ quantifies the complexity of system A with respect to that of an 'a priori' or reference system B. An appropriate symmetrization of the composing factors will allow us to consider the relative complexity among A and B, avoiding the use of an a priori reference in order to deal with a 'distance in complexity', in some sense. To define $C(A,B)$ in this way, let us consider the two factors of the complexity itself $C(A)$, building up then the relative complexity $C(A,B)$ in terms of the relative functionals $D(A,B)$ and $H(A,B)$, in a similar way as done in Ref. [34]:

$$D(A,B) \equiv \frac{D_{AB}}{\sqrt{D_{AA}D_{BB}}} = \frac{\int \rho_A \rho_B d\vec{r}}{\sqrt{\int \rho_A^2 d\vec{r} \int \rho_B^2 d\vec{r}}} \tag{5}$$

is the relative disequilibrium of A with respect to B, and

$$H(A,B) \equiv \exp\left\{\frac{1}{2}[KL(A,B) + KL(B,A)]\right\} \tag{6}$$

is the relative exponential entropy, given in terms of the relative or Kullback–Leibler entropy [36]

$$KL(A,B) \equiv \int \rho_A \ln \frac{\rho_A}{\rho_B} d\vec{r}, \tag{7}$$

widely employed in a huge variety of applications [37–39].

Let us notice that the definition of $D(A,B)$ in Eq. (5) provides a symmetric functional 'per se', being identical to the so-called 'quantum similarity index' $QSI(A,B)$ [18], a measure of similarity among density functions introduced in the early eighties within a chemical framework and later applied in many different fields [40–44]. Its main properties allows to be considered as a measure of distance among probability distributions. Let us remark that the QSI values are restricted to the finite interval $[0,1]$, with $QSI(A,B) = 1$ only for $A = B$.

A straightforward definition of the factor $H(A,B)$ from that of $H(A)$ is proposed in Ref. [34] by replacing the Shannon entropy in Eq. (3) by the relative entropy $KL(A,B)$. This is done there in such a way because the Shannon entropy $S(A)$ is, apart from a constant, the relative entropy of system A with respect to an uniform distribution for system B.

However, such a definition does not provide a symmetric factor, because $KL(A,B) \neq KL(B,A)$ in general. This fact justifies the symmetrization carried out in Eq. (6), in order to consider $H(A,B)$ as an unbiased measure of relative disorder between systems A and B, and then preserving in the relative complexity $C(A,B)$ the symmetry just achieved for $D(A,B)$.

The main purpose in this section is to provide a generalization of the relative complexity functional $C(A,B) = QSI(A,B)H(A,B)$, by taking advantage of well-known monoparametric generalizations for each of the composing factors QSI and H.

In a recent work [45], the definition of the quantum similarity index $QSI(A,B) = D(A,B)$ given by Eq. (5) has been generalized by means of the 'qth order generalized quantum similarity index' $QSI_q = D_q$:

$$D_q\left(\{\rho_i, \omega_i\}_{i=1}^N\right) \equiv \frac{\int (\rho_1^{\omega_1} \cdots \rho_N^{\omega_N})^q d\vec{r}}{(\int \rho_1^q d\vec{r})^{\omega_1} \cdots (\int \rho_N^q d\vec{r})^{\omega_N}}, \tag{8}$$

with the sum of positive numbers $\sum_{i=1}^N \omega_i = 1$. The generalization includes relevant features: (i) the application for an arbitrary number N of functions, not necessarily $N = 2$ as for QSI, (ii) the order q to enhance/diminish the contribution of the tails and the surroundings of local extrema, and (iii) the weights $\{\omega_i\}$ which control the relative importance of each function within the whole set $\{\rho_i\}$.

For the case of two distributions ($N = 2$) with identical weights ($\omega_1 = \omega_2 = 1/2$), the generalized similarity index reads as

$$D_q(A,B) = \frac{\int (\rho_A \rho_B)^{q/2} d\vec{r}}{\sqrt{\int \rho_A^q d\vec{r} \int \rho_B^q d\vec{r}}}, \tag{9}$$

which includes the similarity $QSI = D$ in Eq. (5) for the particular case $q = 2$. The generalized $QSI_q = D_q$ preserves, for arbitrary q, the relevant properties of QSI.

Let us now focus on the disorder/uncertainty factor $H(A,B)$, expressed in Eq. (6) in terms of Kullback–Leibler entropies KL. The KL functional is a limiting case of the so-called 'relative Rényi entropy' [46] of order t

$$R_t(A,B) \equiv \frac{1}{t-1} \ln \int \frac{\rho_A^t}{\rho_B^{t-1}} d\vec{r}, \tag{10}$$

so that $KL(A,B) = R_1(A,B)$. Then, the $H(A,B)$ symmetrized factor admits the generalization

$$H_t(A,B) \equiv \exp\left\{\frac{1}{2}[R_t(A,B) + R_t(B,A)]\right\} \tag{11}$$

verifying $H_1(A,B) = H(A,B)$. A further generalized measure $H_t(\{\rho_i, \omega_i\}_{i=1}^N)$ of weighted relative uncertainty can be defined from an appropriate combination of relative Rényi entropies.

Now we are ready to define a two-parametric relative complexity from the joint use of the two generalized factors described above:

$$C_{q,t}(A,B) \equiv D_q(A,B)H_t(A,B), \tag{12}$$

for any $q, t > 0$ whenever the involved integrals converge. Attending to the descriptions provided below, the quantity $C_{q,t}(A,B)$ constitutes a generalized measure of complexity among distributions. Some comments are in order:

(i) The identity $C_{q,t}(A,A) = 1$ holds for any orders q, t. This means that the relative complexity among a given system and itself is 1.
(ii) The particular case $C_{2,1}(A,B)$ corresponds to the LMC-like relative complexity, with QSI as the first factor and the exponential of the mean KL as the second one. Relevant properties verified by $C_{2,1}(A,B)$ (e.g. invariance under translation and rescaling transformations) are preserved in $C_{q,t}(A,B)$.
(iii) The generalization can be straightforwardly extended by considering a number of functions higher than two, as well as by including arbitrary weights for each of them.

The just introduced definition can be applied to the study of complexity for arbitrary probability distributions. Let us keep in mind that the methodology employed throughout this section is universal, having its grounds in the use of well-known mathematical techniques and information-theoretical functionals.

Next section is devoted to the analysis of the generalized relative complexity among the probability distributions arising from the electron charge density of neutral atoms, through the whole Periodic Table. This kind of study has been carried in the past by using both the complexity itself [23,32,33,47,48], and more recently by means of the relative complexity [34]. In those cases, as also in next section, computations are carried out within a Hartree–Fock framework [49,50]. Atomic units (a.u.) are used throughout.

3. Numerical analysis with atomic electron charge densities

Accordingly with the interpretation of the complexity and the relative complexity as measures of structure, we wonder about the possible connection among their values for atomic systems and their main physical properties. Let us mention that recent studies were carried out, by using the LMC complexity and a variety of other complexities as well [23,25,29–33,47,48] (e.g. Fisher–Shannon, Cramér–Rao or Rényi-like ones). A clear evidence of the aforementioned connection is provided, mainly in terms of the atomic shell-filling patterns, for both neutral and ionized atomic species.

More recently, a similar interpretation has been provided for the LMC-like relative complexity measure $C(A,B)$ proposed in Ref. [34]. The numerical study was performed there as follows: first the system A is chosen as the initial element when filling a given subshell (of 'p', 'd' or 'f' type), and then system B 'runs' over the

subshell, starting with $B = A$ until the subshell is completely filled, that is, when B becomes a closed-subshell system.

We give here a summary of the main conclusions derived from that work: (i) for each subshell, characterized by the reference system A, the initial value is $C(A, B = A) = 1$, (ii) the relative complexity $C(A,B)$ increases monotonically as far as B runs over the subshell, and (iii) the rate of such an increase becomes progressively smaller for subshells with heavier atoms, as compared to that of lighter ones.

Consequently, the only evidence of periodicity, as displayed in the figures enclosed in Ref. [34], arises from the choice 'ad hoc' of the reference systems, namely, just those enclosing a new subshell as compared to the previous element, throughout the whole Periodic Table for neutral atoms with nuclear charges $Z = 1-103$.

We have extended the previous study, at a first step, by choosing one of the aforementioned reference systems, namely Boron (system A with $Z_A = 5$, the initial one as filling the $2p$ subshell), but considering B running all over the Periodic Table ($Z_B = 1-103$), instead of constraining A and B to the same subshell. The results obtained in this way for $C_{q,t}(A,B)$ are displayed in Figure 1a and b, as curves in red for the values $(q,t) = (2,1)$.

Some comments are in order: (i) the results are roughly the same independently of using for $C(A,B)$ the unsymmetrized definition of Ref. [34] or the symmetrized one $C_{2,1}(A,B)$ as in the present work, (ii) the aforementioned monotonic behavior is clearly observed when both A and B have the same valence subshell ($Z_B = 5-10$), and (iii) for most systems with different valence subshell, the relative complexity falls below unity.

Last comment is extremely important, in order to consider (or not) $C(A,B)$ as an appropriate measure of relative complexity. For a pair of systems A and B with relative complexity lower than 1, and keeping in mind that $C(A,A) = 1$, we get the inequality $C(A,B) < C(A,A)$ for many elements B, This inequality holds not only for the illustrative example $Z_A = 5$, but for any other Z_A also.

Considering complexity, in this context, as a measure of structure and organization of the underlying distribution, the inequality $C(A,B) < C(A,A)$ introduces a strong difficulty from a conceptual point of view, as clarified by the following comment: 'the relative complexity of A with respect to B is lower than that of A with respect to itself'. This reading of the above inequality forbides to consider $C(A,B)$ as a measure of structure in B as compared to that
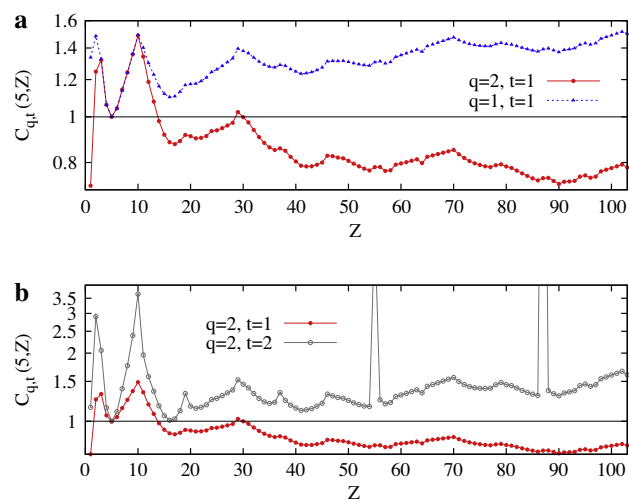
Figure 1. Comparison among the electron charge density of Boron (nuclear charge $Z' = 5$) and those of all neutral atoms with $Z = 1-103$, by means of the generalized relative complexities $C_{q,t}(Z,Z')$ with indexes $t = 1$ and $q = 2$ (in red), and also replacing one of them by (a) $q = 1$ (in blue), and (b) $t = 2$ (in grey). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

of A. In this sense, one should expect to obtain, for fixed A, the minimizer of the relative complexity $C(A,B)$ for $B = A$ or, in other words, the inequality $C(A,A) \leqslant C(A,B)$, with the equality being reached if and only if $A = B$.

This interpretation is used, in fact, within the comments on the results obtained in Ref. [34] for systems belonging to the same subshell, then interpreting $C(A,B)$, in some sense, as a measure of 'distance in complexity' of A from B. The results displayed in Figure 1 provide us with the evidence that such an interpretation fails, in general, when dealing with systems from different subshells.

Let us now consider the generalization $C_{q,t}(A,B)$ of the relative complexity. All previous discussions on the behavior of the red lines for $C(A,B)$ regard, in fact, the particular case $q = 2$ and $t = 1$. The difficulties arising from this choice of (q,t) have been corroborated, unless restricting the analysis to systems with identical valence subshell. We wonder now about the existence of (q,t) values, different from $(2,1)$, allowing us to avoid the previous difficulties. The answer regarding their existence is affirmative, as shown by the blue and grey lines in Figures 1a and 1b, respectively. The generalized relative complexity $C_{1,1}(A,B)$ is considered in Figure 1a, enclosing the similarity factor QSI_1 instead of the QSI one. It is observed that the measure $C_{1,1}(A,B)$ never crosses the unity frontier for the illustrative example here considered, as also occurs for the rest of systems in the Periodic Table. The same conclusion arises from the analysis of $C_{2,2}(A,B)$ in Figure 1b, where the exponential of the symmetrized relative Rényi entropy of order $t = 2$ replaces the limiting factor KL corresponding to $t = 1$.

Consequently, it is numerically observed that the generalized comparative functionals $C_{1,1}(A,B)$ and $C_{2,2}(A,B)$ comply with the desirable properties for a measure of relative complexity, contrary to the pioneering $C(A,B) \sim C_{2,1}(A,B)$ one. In addition, the display of numerous local extrema in all curves is related to the atomic shell structure of the systems under comparison, as will be discussed later.

And, what about other arbitrary (q,t) values? For several pair of systems, with nuclear charges Z_A and Z_B, a plane substended by q and t has been drawn, according to the condition $C_{q,t}(A,B) \geqslant 1$. The condition divides the plane into two regions, the 'allowed' and 'forbbiden' ones. An illustrative example is provided in Figure 2 for systems $Z = 5,17$. The upper area, in color, is the allowed region when dealing with the (q,t)-generalized relative complexity. Let us notice the star in the white forbidden area, located at $(q = 2, t = 1)$, i.e. just the values corresponding to the particular case $C(A,B)$ as defined in Ref. [34].

Other planes for different pairs of atomic systems have been also analyzed. The main comments regarding all those planes are: (i) the shape of the frontier between the aforementioned regions strongly depends on the choice of systems, most usually
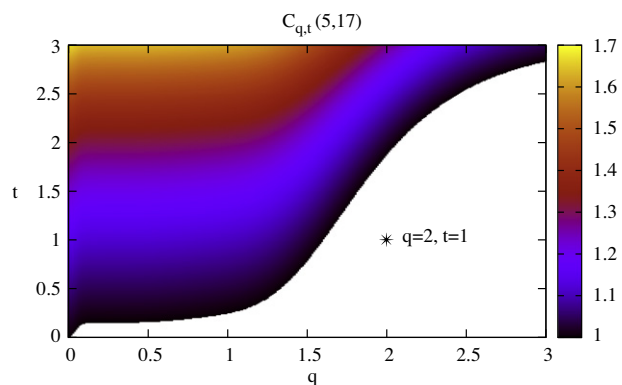
because of their shell structure, and (ii) in spite of the different shapes, a common feature is the existence of thresholds, which translate into the condition $t > t_{min}(q)$ for a given q.

It still remains the problem of determining a rigorous (and desirable) analytical condition on the parameters (q,t) in order to guarantee that the value of the relative complexity between two arbitrary distributions is not below 1. Nevertheless, some achievements are noteworthy:

- for the particular case $q = 1$, the inequality $C_{1,t}(f,g) \geqslant 1$ holds with arbitrary probability distributions f,g for any $t \geqslant 1/2$ (as far as the integrals involved converge); in particular, we have proven the existence of a value $0 < t_{min} \leqslant 1/2$ so that the condition reads as $t \geqslant t_{min}$,
- for ground-state n-dimensional hydrogenic atoms (one-electron systems), with respective nuclear charges Z_A and Z_B, the above inequality is fulfilled for arbitrary $q > 0$ and $1/4 \leqslant t \leqslant \max\{Z_A, Z_B\}/|Z_A - Z_B|$. Let us remark that this condition (i) depends upon the nuclear charges through their quotient Z_A/Z_B, and (ii) does not depend on the dimensionality n.

Continuing with the numerical analysis of the atomic relative complexity, we compare now two curves of $C_{1,1}(Z',Z)$ throughout the Periodic Table ($Z = 1-103$), for Z' corresponding to extremely similar (Figure 3a) or different (Figure 3b) systems from a physical and chemical point of view. As an illustrative example, two noble gases are chosen in Figure 3a: Helium ($Z' = 2$) and Neon ($Z' = 10$). In spite of the differences based on their absolute values, the curves $C_{1,1}(2,Z)$ and $C_{1,1}(10,Z)$ display a very similar structure, accordingly with the fact that both Helium and Neon belong to the same group of the Periodic Table. In this sense, it is worthy to mention that they share most local minima, at $Z = 2,10,18,24,29,36,42,46,54$, as well as the close ones $Z = 78-79$ for Helium and Neon, respectively. Let us notice that the list encloses (i) the noble gases $Z = 2,10,18,36,54$, and (ii) systems suffering from the anomalous shell-filling: $Z = 24,29,42,46,78-79$. So, the value of the relative complexity provides information on relevant features regarding the shell-structure of the systems compared.

We find just the opposite behavior when dealing with two systems as different as Helium (noble gas, $Z' = 2$) and Beryllium (alkaline-earth, $Z' = 4$), as shown in Figure 3b. While different minima of Helium's curve occurs for the comparison with other noble
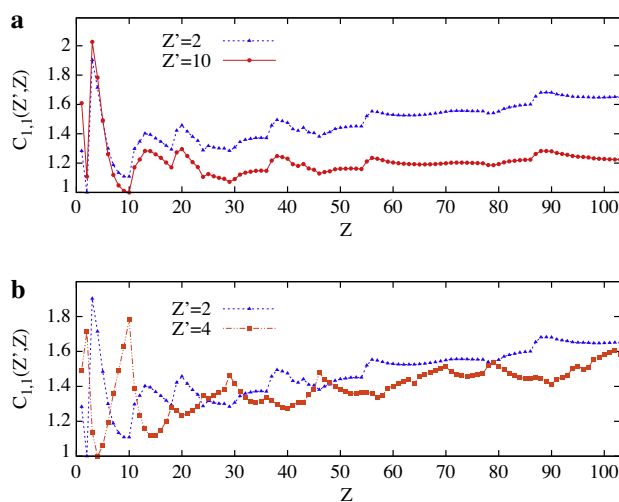

Figure 3. Generalized relative complexity $C_{1,1}(Z,Z')$, for $Z = 1 - 103$, and (a) two noble gases (Helium and Neon, $Z' = 2,10$), and (b) a noble gas (Helium, $Z' = 2$) and an alkaline-earth (Beryllium, $Z' = 4$).

Figure 2. Region (colored) in the (q,t) plane where the generalized relative complexity between Boron ($Z = 5$) and Chlorine ($Z = 17$) verifies $C_{q,t}(5,17) \geqslant 1$.

Table 1
Generalized relative complexity $C_{2,1}(nl)$ among the electron densities of all neutral atoms filling the subshell characterized by the quantum numbers (n,l).

Subshell n,l	$C_{2,1}(nl)$
2p	1.448005
3p	1.192296
3d	1.152400
4p	1.046343
4d	1.102025
5p	1.024107
4f	1.065817
5d	1.028909
6p	1.010805
5f	1.045200

gases, the same comment applies for alkaline-earths with respect to Beryllium. In fact, most minima for one system corresponds to maxima of the other, and conversely. For instance, systems $Z = 2, 10, 18, 24, 29, 36, 42, 46$ are minima of Helium and maxima of Beryllium. Additionally, the same occurs for the close ones $Z = 54 - 55, 62 - 63, 78 - 79$. As discussed previously, most of them are either noble gases or systems with anomalous shell-filling. But now, they are displayed as minima or maxima depending on the performance of a comparison with a noble gas or an alkaline-earth.

Similar comments to those here provided apply also for the numerical study by choosing other different groups of the Periodic Table. The shell-filling patterns are clearly displayed, as provided by the location of local maxima or minima for the curves considered.

To conclude the numerical study, we provide here an application of the relative complexity among a set of systems. In doing so, we consider the filling process of the different atomic subshells. In Ref. [34], this kind of analysis is carried out in terms of the 'one-to-one' relative complexity, by fixing a reference system as the initial one of a given subshell, the second one running over such a subshell. Here, instead, we consider the relative complexity among all systems belonging to the same subshell. For illustration, uniform weights are chosen for both factors of the relative complexity, namely QSI_q and the exponential of relative Rényi entropies between each density within the set and their arithmetic mean (the mean obtained by employing uniform weights also). Nevertheless, different criteria could be considered in order to establish the weights, such as e.g. relative number of electrons, masses or sizes.

The results obtained are shown in Table 1. It is observed a rough decreasing trend of the values, as far as heavier systems are considered. This comment is in accordance with those regarding the aforementioned analysis in Ref. [34], where the relative complexity with respect to the initial system increases through the subshell, but at a progressively slower rate. This means that differences in terms of relative complexity become smaller for heavy systems as compared to the lighter ones, as induced from the results on that work and the present one.

Deviations from the decreasing trend occur for subshells 3d, 4f and 5f. These subshells contain a relevant number of elements with anomalous shell-filling. Their high values of relative complexity are interpreted according to a mix of elements with relevant differences regarding their shell-structure. This fact is clearly revealed in the values of Table 1. Let us point out that these comments, regarding relative complexities of whole subshells, also hold for other values of the parameters q and/or t.

4. Conclusions and open problems

In order to define an appropriate measure of relative complexity among two or more distributions, it is essential to take into ac-

count the desirable properties which should be verified. This is so because of the aim of dealing with a physically meaningful measure. Such is not the case of the pioneering definition, which leads to a contradictory interpretation from a conceptual point of view.

Those difficulties can be avoided by dealing with the generalized relative complexity defined in the present work. Furthermore, this generalization allows to introduce the concept of relative complexity among an arbitrary number of functions, with the option of considering different weights for each of them.

The numerical analysis for the comparison of two neutral atoms, located anywhere at the Periodic Table, has allowed us to provide a clear interpretation in terms of a so relevant feature of atomic systems as their shell structure is. This kind of interpretation is even more efficient when expressed in terms of the different groups which the systems belong to. In this sense, it is worthy to remark that these groups are characterized by the main physical and chemical atomic properties.

There are several open problems regarding both the definition and applications here considered. Let us remark the following: (i) the determination of rigorous conditions on the characteristic parameters in order to guarantee values of the relative complexity not below unity, and (ii) the application to more sophisticated systems (e.g. molecules), physical processes (ionization, excitation), distributions (e.g. momentum space) or models (relativistic effects, configuration interactions).

Acknowledgements

References

[1] P. Bernaola-Galván, I. Grosse, P. Carpena, J.L. Oliver, R. Román-Roldán, H.E. Stanley, Phys. Rev. Lett. 85 (2000) 1342.
[2] G. Chechik, V. Sharma, U. Shalit, S. Bengio, J. Mach. Learn. Res. 11 (2010) 1109.
[3] P. Faratin, C. Sierra, N.R. Jennings, Artif. Intell. 142 (2002) 205.
[4] C. Zhang, H. Fu, Pattern Recognit. Lett. 27 (2006) 1307.
[5] A.P. Majtey, P.W. Lamberti, D.P. Prato, Phys. Rev. A 72 (2005) 052310.
[6] P.W. Lamberti, A.P. Majtey, A. Borrás, M. Casas, A. Plastino, Phys. Rev. A 77 (2008) 052311.
[7] R.O. Esquivel, N. Flores-Gallegos, M. Molina-Espíritu, A.R. Plastino, J.C. Angulo, J. Antolín, J.S. Dehesa, J. Phys. B: At. Mol. Opt. Phys. 44 (2011) 175101.
[8] J.S. Dehesa, A. Martínez-Finkelshtein, V.N. Sorokin, Mol. Phys. 104 (2006) 613.
[9] P.A. Bouvrie, J.C. Angulo, J.S. Dehesa, Physica A 390 (2011) 2215.
[10] S.R. Gadre, R.D. Bendale, S.P. Gejji, Chem. Phys. Lett. 17 (1985) 138.
[11] M. Ho, V.H. Smith Jr., D.F. Weaver, C. Gatti, R.P. Sagar, R.O. Esquivel, J. Chem. Phys. 108 (1998) 5469.
[12] S. Janssens, A. Borgoo, C. van Alsenoy, P. Geerlings, J. Phys. Chem. A 112 (2008) 10560.
[13] S. López-Rosa, J. Antolín, J.C. Angulo, R.O. Esquivel, Phys. Rev. A 80 (2009) 012505.
[14] S. López-Rosa, R.O. Esquivel, J.C. Angulo, J. Antolín, J.S. Dehesa, N. Flores-Gallegos, J. Chem. Theory Comput. 6 (2010) 145.
[15] C.E. Shannon, W. Weaver, The Mathematical Theory of Communication, University of Illinois Press, Urbana, 1949.
[16] R.A. Fisher, Proc. Cambridge Philos. Soc. 22 (1925) 700.
[17] J. Pipek, I. Varga, Phys. Rev. A 46 (1992) 3148.
[18] R. Carbó-Dorca, J. Arnau, L. Leyda, Int. J. Quant. Chem. 17 (1980) 1185.
[19] J. Antolín, J.C. Angulo, S. López-Rosa, J. Chem. Phys. 130 (2009) 074110.
[20] K.D. Sen (Ed.), Statistical Complexity. Applications in Electronic Estructure, Springer, London, 2011.
[21] C.R. Shalizi, K.L. Shalizi, R. Haslinger, Phys. Rev. Lett. 93 (2004) 118701.
[22] O.A. Rosso, M.T. Martin, A. Plastino, Physica A 320 (2003) 497.
[23] K.Ch. Chatzisavvas, Ch.C. Moustakidis, C.P. Panos, J. Chem. Phys. 123 (2005) 174111.
[24] R. López-Ruiz, H.L. Mancini, X. Calbet, Phys. Lett. A 209 (1995) 321.
[25] T. Yamano, J. Math. Phys. 45 (2004) 1974.
[26] R.O. Esquivel, J.C. Angulo, J. Antolín, J.S. Dehesa, S. López-Rosa, N. Flores-Gallegos, Phys. Chem. Chem. Phys. 12 (2010) 7108.
[27] J.S. Shiner, M. Davison, P.T. Landsberg, Phys. Rev. E 59 (1999) 1459.
[28] D. Feldman, J.P. Crutchfield, Phys. Lett. A 238 (1998) 244.
[29] X. Calbet, R. López-Ruiz, Phys. Rev. E 63 (2001) 066116.

[30] M.T. Martin, A. Plastino, O.A. Rosso, Physica A 369 (2006) 439.
[31] J. Antolín, S. López-Rosa, J.C. Angulo, Chem. Phys. Lett. 474 (2009) 233.
[32] K.D. Sen, J. Antolín, J.C. Angulo, Phys. Rev. A 76 (2007) 032502.
[33] J.C. Angulo, J. Antolín, J. Chem. Phys. 128 (2008) 164109.
[34] A. Borgoo, P. Geerlings, K.D. Sen, Phys. Lett. A 375 (2011) 3829.
[35] E. Romera, K.D. Sen, A. Nagy, J. Stat. Mech. (2011) P09016.
[36] S. Kullback, A. Leibler, Ann. Math. Statist. 22 (1951) 79.
[37] M. Ho, R.P. Sagar, H. Schmider, D.F. Weaver, V.H. Smith Jr., Int. J. Quantum Chem. 53 (1995) 627.
[38] R.P. Sagar, N.L. Guevara, J. Mol. Struct. (THEOCHEM) 857 (2008) 72.
[39] A. Borgoo, P. Jaque, A. Toro-Labbé, C. van Alsenoy, P. Geerlings, Phys. Chem. Chem. Phys. 11 (2009) 476.
[40] R. Carbó-Dorca, X. Gironés, P.G. Mezey (Eds.), Fundamentals of Molecular Similarity, Kluwer Academic/Plenum Press, New York, 2001.

[41] J. Cioslowski, A. Nanayakkara, J. Am. Chem. Soc. 115 (1993) 11213.
[42] D. Robert, R. Carbó-Dorca, Int. J. Quantum Chem. 77 (2000) 685.
[43] A. Borgoo, M. Godefroid, K.D. Sen, F. de Proft, P. Geerlings, Chem. Phys. Lett. 399 (2004) 363.
[44] N.L. Allan, D.L. Cooper, J. Math. Chem. 23 (1998) 51.
[45] P.A. Bouvrie, J. Antolín, J.C. Angulo, Chem. Phys. Lett. 506 (2011) 326.
[46] A. Nágy, E. Romera, Int. J. Quantum Chem. 109 (2009) 2490.
[47] C.P. Panos, K.Ch. Chatzisavvas, Ch.C. Moustakidis, E.G. Kirkou, Phys. Lett. A 363 (2007) 78.
[48] A. Borgoo, F. De Proft, P. Geerlings, K.D. Sen, Chem. Phys. Lett. 444 (2007) 186.
[49] T. Koga, K. Kanayama, S. Watanabe, A.J. Thakkar, Int. J. Quantum Chem. 71 (1999) 491.
[50] T. Koga, K. Kanayama, S. Watanabe, T. Imai, A.J. Thakkar, Theor. Chem. Acc. 104 (2000) 411.