Rigorous properties and uncertainty-like relationships on product-complexity measures: Application to atomic systems

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A B S T R A C T

Most of research on complexities and the corresponding conclusions have been obtained by numerically quantifying their values, and little attention has been paid to their theoretical properties and the exact meaning within an statistical framework, valid for any arbitrary n-dimensional distribution. In the present work, different product-complexities, constructed as a product of two relevant information quantities associated to the concepts of uncertainty and localization are investigated. Different results on product-complexities, such as rigorous bounds, uncertainty-like inequalities, relationships among themselves and also statistical interpretations are given. For the sake of completeness, some of these analytical results on product-complexities are numerically checked for the one-particle densities of atomic systems in both conjugated spaces.

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1. Introduction

The interest in the concept of *complexity* is growing due to its proven usefulness in order to better describe, in terms of distribution functions, the level of organization of a system or process in many diverse fields of science. There exist different definitions of complexity, each possessing its own properties which make it more or less appropriate depending on the kind of phenomenon under study.

The starting point for finding the origin of the concept of *complexity* for an arbitrary system or process is, in fact, difficult to establish, because such a magnitude has appeared as a fundamental quantity when dealing with the problem of quantifying the content of 'information' or 'localization' in many different fields of science.

Complexity measures are proposed as general indicators of pattern, structure and correlation in systems or processes. Many alternative mathematical frameworks exist for quantifying the notions of complexity or information, including the Kolmogorov–Chaitin or algorithmic information theory [1,2], classical information theory of Shannon and Weaver [3], the Fisher information [4,5], logical depth [6], computational mechanics [7] and others [8–11]. Most share formal similarities with the others as well as with Bayes and Information Theory [12].

Indeed, the term complexity has many different meanings and adjectives (algorithmic, geometrical, computational, stochastic, effective, structural, statistical, excess entropy) and is used in very different fields (dynamical systems, time series, quantum wave functions in disordered systems, spatial patterns, language, analysis of multi-electronic systems, cellular automata, neuronal networks, self-organization, molecular or DNA analyses, social sciences, etc.) [13–15]. Although there is no general agreement about the definition of what complexity is, its quantitative characterization is a very important subject of research in nature and has received considerable attention over the past years [16,17].

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Therefore the characterization of complexity cannot be univocal and must be adequate for the type of structure or process we study, the nature and the goal of the description we want and for the level or scale of the observation that we use. In the same way it is interesting to combine the properties of the new proposals to characterize complexity and test them on diverse and known physical systems or processes.

Fundamental concepts such as information or entropy are frequently present in the proposals for characterizing complexity, but some other ingredients that do not only capture uncertainty or randomness can also be searched. One wishes also to capture some other properties such as clustering, order or organization of the systems or process.

Some of the definitions and relations between the above concepts are not clear; even less so is how disorder or randomness takes part in the aforementioned properties of the system and vice versa.

The initial form of complexity is designed such that it vanishes for the two extreme probability distributions (little complex ones), corresponding to perfect order (represented by a Dirac-delta) and maximum disorder (associated with a highly flat distribution). Most of those definitions take into account elements of Bayesian and information theories. Some of the more recent ones consist of the product of two factors, measuring, respectively, order and disorder on the given systems or, equivalently, localization and delocalization [18,19]. They will be referred to as product-complexities.

Even restricting ourselves to the aforementioned factorization, there is no unique definition for complexity. The reason is that there exist different candidates for being one of the coupled factors which give rise to complexity. The most popular ones are well-known to play a relevant role in an information-theoretic framework. Among them, let us mention the Shannon entropy S, the disequilibrium D, the Fisher information I and the variance V. Much work has been done using those quantities as basic measures, not only for quantifying the level of spreading of distributions but also for many other applications, such as, for instance, maximum-entropy estimation and reconstruction of an unknown distribution from very limited information on it.

The measures mentioned above are defined for an arbitrary n-dimensional distribution $\rho(\mathbf{r})$, where normalization is given by

$$\int \rho(\mathbf{r})d\mathbf{r} = 1 \tag{1}$$

and the integration is performed over the n-dimensional space $\mathbb{R}^n$. Consequently, the vector $\mathbf{r}$ consists of n components, which can be expressed equivalently in cartesian of spherical coordinates, namely $\mathbf{r} = (x_1, \ldots, x_n) = (r, \theta_1, \ldots, \theta_{n-2}, \phi)$, where $r = |\mathbf{r}|$ is the modulus of the spatial vector.

It is customary to deal additionally with the corresponding distribution in the so-called *conjugated space*. This is the case in which the $\mathbf{r}$-space distribution is defined from an initial wavefunction $\Psi(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N)$ by integrating $|\Psi|^2$ on all variables except $\mathbf{r}$. If one considers the Fourier transform $\tilde{\Psi}(\mathbf{p}, \mathbf{p}_2, \ldots, \mathbf{p}_N)$ to build up the associated distribution $\gamma(\mathbf{p})$ (preserving normalization), many properties and characteristics of both densities $\rho(\mathbf{r})$ and $\gamma(\mathbf{p})$ are well-known to be strongly related. Such is the case, for instance, of the so-called *one-particle densities* of many-particle systems (e.g. atoms, molecules), in which $\rho(\mathbf{r})$ quantify the mass density around location $\mathbf{r}$ and $\gamma(\mathbf{p})$ the linear momentum distribution around the momentum vector $\mathbf{p}$. Different relationships involving quantities associated to both complementary densities are of capital importance through the concept of *uncertainty* of the system.

For illustration, an analysis of different relationships among information-theoretic quantities will be carried out in the present work for a large set of atomic systems. For such a particular case we will deal with densities whose domain are the three-dimensional ($n = 3$) space. Studies on complexity has been also done in previous works, mainly by computing their numerical values [15], unlike the present work where rigorous relationships among different complexities and/or other information magnitudes are obtained, which are valid for arbitrary systems and dimensionalities.

In what follows, atomic units (a.u.) will be considered for variables, densities, functionals and complexities (i.e. $\hbar = |m| = e = 1$ and, consequently, also the Bohr radius $a_0 = 1$) when carrying out the numerical analysis for atomic systems. Fixing the system of units is essential for a proper description of different quantities, according to their definition.

It is also worth mentioning that: (i) the product distribution $f(\mathbf{r}, \mathbf{p}) \equiv \rho(\mathbf{r})\gamma(\mathbf{p})$ will be also considered in order to have a more complete informational description of the system; (ii) in some cases (e.g. atomic systems), it will be sufficient to deal with the spherically averaged densities $\rho(r)$ and $\gamma(p)$, for which the independent variable range is the non-negative real line $[0, \infty)$.

This paper is structured as follows. In Section 2, information measures and complexities we deal with are defined for arbitrary distributions and dimensionalities. Section 3 is devoted to obtaining new properties and statistical interpretations of the different studied complexities; some of them are also numerically analysed for one-particle atomic densities. In Section 4, it is shown how different complexities are also related among themselves by means of uncertainty-like products, and in Section 5, the role of complexity in the problem of information extremization is considered in the general case, emphasizing the analytical results for hydrogenic systems. Finally, some conclusions are given.

2. Information and product-complexity measures

Many different information measures are known to play a relevant role when studying the level or content of information within an arbitrary distribution or a process, most of them expressed as density functionals. This is, for instance, the case of

the Shannon entropy [3] of $\rho(\mathbf{r})$, defined as

$$S_r \equiv - \int \rho(\mathbf{r}) \ln \rho(\mathbf{r}) d\mathbf{r}, \tag{2}$$

the Fisher information, given by [4]

$$I_r \equiv \int \rho(\mathbf{r}) |\vec{\nabla} \ln \rho(\mathbf{r})|^2 d\mathbf{r}, \tag{3}$$

the variance [20]

$$V_r \equiv \langle r^2 \rangle - \langle r \rangle^2 \tag{4}$$

which is defined in terms of radial expectation values $\langle r^k \rangle \equiv \int r^k \rho(\mathbf{r}) d\mathbf{r}$, and the frequency or entropic moments [21]

$$\omega_r(q) \equiv \int \rho^q(\mathbf{r}) d\mathbf{r}, \tag{5}$$

strongly related to the so-called Renyi [22] and Tsallis [23] entropies, $R_r(q)$ and $T_r(q)$ respectively, as

$$R_r(q) = \frac{\ln \omega_r(q)}{1 - q} \tag{6}$$

$$T_r(q) = \frac{1 - \omega_r(q)}{q - 1}, \tag{7}$$

and similarly for the corresponding quantities in momentum and product spaces (denoted with the subscripts 'p' or 'rp' instead of 'r') by only replacing $\rho(\mathbf{r})$ by $\gamma(\mathbf{p})$ or $f(\mathbf{r}, \mathbf{p})$. At times, we will omit subscripts in equations and definitions, understanding their validity for any arbitrary space.

It is worth mentioning that (i) the limiting case $q = 1$ corresponds for both the Renyi and the Tsallis entropies (in all spaces) to the Shannon one S, i.e. $R(1) = T(1) = S$, and (ii) a specially interesting case within the information theory framework is given by the second-order frequency moment, denoted by

$$D \equiv \int \rho^2(\mathbf{r}) d\mathbf{r} \tag{8}$$

and being known as *disequilibrium* (and also as information energy or self-similarity) [18,24–26], because provides information on the closeness of the function to the uniform distribution.

The three complexities we are going to deal with in the present work are built up in terms of some of the above defined quantities. Apart from these complexities, additional ones have been also considered in the literature (e.g. SDL complexity [19] or $D \cdot V$ and $I \cdot L$ products [27]). Nevertheless, we will focus on the study of those three because they have been very recently shown to be strongly related to different structural properties of many-fermion systems, specially when working simultaneously with both position and momentum conjugated variables [28,29,27]. They are defined as follows:

1. López-Ruiz, Mancini and Calbet complexity $C(LMC)$: In its original form [18], it was defined as the product of the disequilibrium D and the Shannon entropy S, as components associated with the concepts of localization and delocalization, respectively.

   After some modifications attending to the desirable properties of complexities (e.g. invariance under replication, translation and rescaling transformations), the final form for the LMC complexity, as being also considered throughout this work, is [18,16,30–33]

   $$C(LMC) \equiv D \cdot L \equiv D \cdot e^S, \tag{9}$$

   where, for convenience, the exponential entropy $L = e^S$ has been also introduced.

   The usefulness of this complexity has been checked in many fields [14,15,31] and allows for reliable detection of periodic, quasiperiodic, linear stochastic and chaotic dynamics [18,31,32].

   Its definition allows one to observe the aforementioned small values for extreme distributions, because the Shannon entropy approaches $-\infty$ for highly concentrated distributions (and consequently $L \to 0$), while the disequilibrium goes to zero as the distribution spreads uniformly over its domain.

   Numerous studies on $C(LMC)$ have been carried out in order to better understand the structural characteristics of the analyzed distribution. Most of such studies have been done attending to the numerical values displayed by the $C(LMC)$ complexity for specific distributions, each one having its own characteristics. However, it would be also very useful to have at our disposal rigorous properties on such a measure, applicable to arbitrary density functions.

   Contrary to the case of the isolated factors which define $C(LMC)$, namely, the disequilibrium and the exponential Shannon entropy, not many rigorous properties and/or relationships are known on complexity. Concerning the aforementioned factors, it is worthy to mention, among others, the variational upper and/or lower bounds on each factor in terms of radial expectation values of the density [34,35].

2. Fisher–Shannon complexity $C(FS)$: In this case, we have recently introduced [28,29] a complexity composed of two significantly different factors, namely a *local* one as the Fisher information I and a *global* one known as 'power entropy' J, namely

$$C(FS) \equiv I \cdot J \tag{10}$$

where

$$J \equiv \frac{1}{2\pi e} e^{\frac{2}{n}S}. \tag{11}$$

Both quantities determine the so-called *Fisher–Shannon plane*, where the definition of the power entropy is based on well-known inequalities on such a product [36].

Here, the role previously played by the disequilibrium is replaced by a local measure as the Fisher information, being the combination of such a two different factors of great utility when dealing with the study of detailed structure.

3. Cramer–Rao complexity $C(CR)$: Cramer–Rao complexity emerges when, as we did in Ref. [27], considering the product of a local and a global measure, involving, on one hand, the Fisher information I as the local one again and, on the other, the variance V of the distribution for measuring the degree of deviation from the mean value. Such a complexity corresponds essentially to the 'Cramer–Rao product', giving rise to [27]

$$C(CR) \equiv I \cdot V \tag{12}$$

for which the inequality $C(CR) \geq n^2$ is also known [36,37].

The same comments made for LMC complexity values of the two extreme cases (i.e. LMC becomes minimal for delta and uniform distributions) are also valid for $C(FS)$ and $C(CR)$, because the Fisher information approaches zero as the distribution spread uniformly over its domain, while both the power entropy and the variance vanishes for Dirac-delta ones.

3. Rigorous properties on complexity measures

In this section, different rigorous properties on the aforementioned complexities will be shown, all valid for arbitrary n-dimensional distributions. In some cases (well known for the Fisher–Shannon and Cramer–Rao complexities), there exist lower bounds given as universal constant values (not necessarily dependent on dimensionality). However, such a value has been only shown to exist for the one-dimensional case [38] (i.e. for densities having as domain the real line), what is generalized for arbitrary dimensionality in the present work. Other results are here expressed as bounds in terms of expectation values and/or density functionals. For the sake of completeness, a numerical analysis will also be carried out for the one-particle densities of atomic systems within a Hartree–Fock framework.

Starting with López-Ruiz, Mancini and Calbet complexity $C(LMC) = D \cdot e^S$, let us firstly observe that it can be also expressed in terms of frequency moments $\omega(q)$. To this end, it is convenient to define the function

$$f(q) \equiv \ln \omega(q) \tag{13}$$

which, due to the normalization constraint, takes the particular value $f(1) = 0$. Additionally, let us write the LMC complexity as $C(LMC) = \exp\{\ln D + S\}$.

Attending to the definition of S and D, it is easy to check that $S = -f'(1)$, i.e. minus the slope of the function $f(q)$ at $q = 1$, and

$$\ln D = \ln \omega(2) = f(2) = \frac{f(2) - f(1)}{2 - 1} \tag{14}$$

where the normalization constraint has been taken into account. Last equality is written in order to point out that $\ln D$ represents the slope of the straight line connecting points of the function $f(q)$ at $q = 1$ and $q = 2$. Finally, and having in mind the convexity of $f(q)$ (or equivalently, the log-convexity of frequency moments $\omega(q)$ as can be easily shown by using Hölder's inequality), it is concluded that the single exponent on $C(LMC)$ written as above is non-negative and, consequently, that $C(LMC) \geq 1$.

To the best of our knowledge, this is the first time that a universal (i.e. valid for any n-dimensional function) constant lower bound on LMC complexity is obtained.

Moreover, from this proof it is immediately concluded that equality $C(LMC) = 1$ is only reached for uniform distributions with a finite volume support. To this end, it is enough to observe that equality is only possible for a linear $f(q)$ over the range $1 \leq q \leq 2$. Such a linearity translates on frequency moments as $\omega(q) = D^{q-1}$ (where the values $\omega(1) = 1$ and $\omega(2) = D$ have been considered). This means that

$$\int \left(\frac{\rho(\mathbf{r})}{D}\right)^q d\mathbf{r} = \frac{1}{D}. \tag{15}$$

The non-dependence on 'q' of the right-hand-side requires the fraction on the integral to take only the values 0 or 1. Then, the density has the constant value $\rho(\mathbf{r}) = D$ on its whole support Λ (appart from, at most, a zero-measure set of points), being the volume of the support $1/D$ in order to keep the normalization condition.
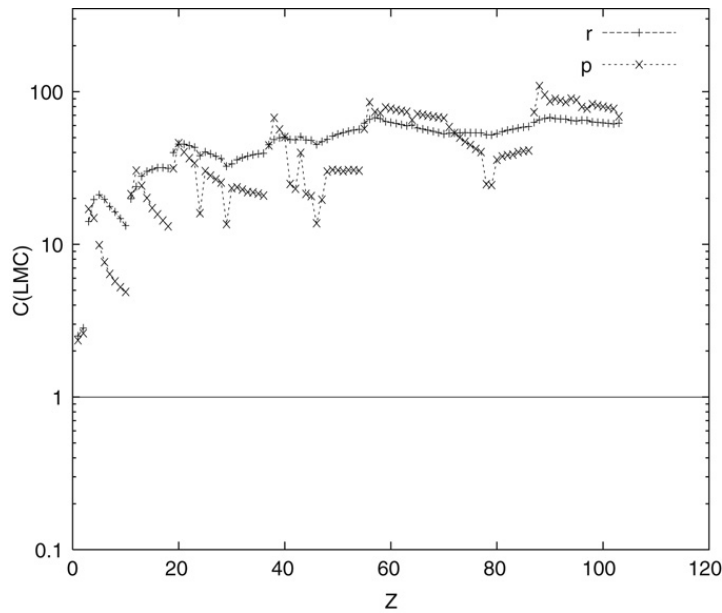
Fig. 1. LMC complexities $C(LMC)$ in position and momentum spaces for neutral atoms with nuclear charge from $Z = 1$ to $Z = 103$. Atomic units (a.u.) are used.

It is remarkable that the lowest LMC complexity corresponds to step distributions over a finite set Λ, which are precisely the maximum-entropy ones among those with domain Λ. They also necessarily minimize the disequilibrium, well-known when dealing with finite-size domains.

In summary, uniform distributions simultaneously minimize the disequilibrium D (i.e. localization) and maximize the Shannon entropy, and consequently the exponential entropy L (i.e. delocalization). But the joint effect of the two opposite ones on each factor of the $C(LMC)$ complexity is dominated by the minimizer one (i.e. the disequilibrium), giving rise to the minimum LMC complexity for uniform densities.

So, it should be expected that the higher $C(LMC)$ values are, the more far from uniformity the density is. To have an idea on the validity of this remark as well as on the comparison of complexity to unity, we show in Fig. 1 the values of LMC complexity of position and momentum densities, $\rho(\mathbf{r})$ and $\gamma(\mathbf{p})$ respectively, for neutral atoms with nuclear charge from $Z = 1$ to $Z = 103$. In doing so, the Near-Hartree–Fock wavefunctions of Koga et al. [39,40] have been employed. The discontinuities in the curves correspond to their decomposition according to the different periods conforming the whole Periodic Table, as also done for drawing the curves in the rest of figures.

It is clearly observed that, apart from being all values in both spaces above unity, there appear different pieces in each curve corresponding to electronic filling of specific subshells, displaying monotonic behaviors which are opposite when comparing both conjugated spaces. This can be interpreted in terms of the uncertainty principle (which will be also analyzed in next sections), in such a way that a higher delocalization in one space is associated to a higher localization in the conjugated one.

Additionally, higher values of complexity for heavy atoms are due to the *lost of uniformity* because of the increase in the level of shell structure, image with exactly corresponds to the intuitive notion of *complexity* of a system.

Let us now concentrate on the Fisher–Shannon complexity $C(FS) = I \cdot J$, in which the localization factor, namely the Fisher information I, has a *local* character, in the sense that it constitutes a sensitive measure of the variation of gradient along the domain of the distribution. Such a measure is of different character than the other component, defined in terms of a global measure as the Shannon entropy.

The inequality $I \cdot J \geq n$ [41], which provides a lower bound to the product of both quantities, is consequently written in terms of the Fisher–Shannon complexity, as

$$C_r(FS) \geq n \tag{16}$$

$$C_p(FS) \geq n \tag{17}$$

$$C_{rp}(FS) \geq 2\pi e n^2, \tag{18}$$

where 'n' is the dimension of the space, and last inequality contains an additional factor apart from the product of complexities in conjugated spaces because of the definition of the power entropy J_{rp} in the product space. It is worth mentioning that the above inequalities are valid for arbitrary distributions on n-dimensional spaces, in the same line as the lower bound $C(LMC) \geq 1$ previously obtained for LMC complexities independently of the space we are dealing with.

The numerical analysis of Fig. 2 for $C(FS)$ is now carried out similarly as done in Fig. 1 for $C(LMC)$, by considering exactly the same systems and spaces. Now, the lower bound is established by the three-dimensional ($n = 3$) space as domain of
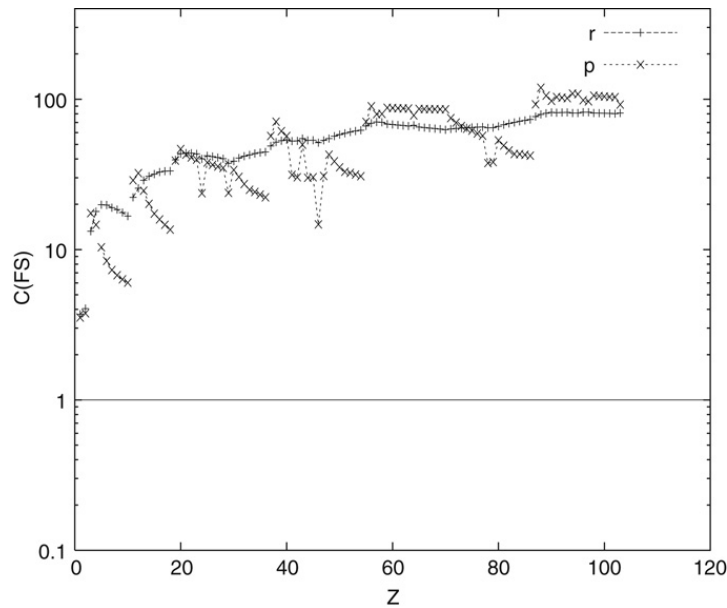
Fig. 2. Fisher–Shannon complexities $C(FS)$ in position and momentum spaces for neutral atoms with nuclear charge from $Z = 1$ to $Z = 103$. Atomic units (a.u.) are used.

the distributions. Similar comments to those of the previous figure, on the behavior in terms of the nuclear charge Z, can be also done.

In spite of the different characteristics of the two main components of the Fisher–Shannon complexity $C(FS) = I \cdot J$, it is known a result which provides a connection between both information measures $I(\rho)$ and $J(\rho)$, which as we will show can also be expressed and interpreted in terms of complexities. The above-mentioned connection arises from the so-called effect of *gaussian perturbation*, and it provides information on the variation suffered by the information content of a distribution ρ when adding a very small gaussian one. Concerning the Fisher and Shannon measures, it is known that

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon} S(\rho + \sqrt{\epsilon}\rho_G)\bigg|_{\epsilon=0} = \frac{1}{2} I(\rho), \tag{19}$$

as shown by de Bruijn [37], where ρ_G denotes the standard gaussian distribution with mean 0 and variance 1. In this sense, the Fisher information could be understood as a measure of the variation of Shannon entropy of the starting density under a gaussian perturbation.

Keeping in mind this result, let us consider the power entropy of the perturbed distribution $\rho_\epsilon \equiv \rho + \sqrt{\epsilon}\rho_G$, namely

$$J(\rho_\epsilon) = \frac{1}{2\pi e} e^{\frac{2}{n} S(\rho_\epsilon)}. \tag{20}$$

Carrying out the same derivation and limiting operations as in Eq. (19), but on the power entropy $J(\rho_\epsilon)$ instead of the Shannon entropy $S(\rho_\epsilon)$, it is immediate to check that

$$C(FS) = n \frac{\mathrm{d}}{\mathrm{d}\epsilon} J(\rho + \sqrt{\epsilon}\rho_G)\bigg|_{\epsilon=0}, \tag{21}$$

what gives rise to an additional interpretation on the Fisher–Shannon complexity: it represents the variation of the power entropy J of a given density ρ when perturbed by a gaussian distribution ρ_G. So, the interpretation of the Fisher information (a single measure of information) according to the process of Gaussian perturbation is now extended to the interpretation, for the same process, in terms of FS complexity (a product-complexity involving simultaneously two information measures).

Concerning the Cramer–Rao complexity $C(CR)$, we next show that it can be also bound from below in terms of radial expectation values of the density. This kind of upper and/or lower bounds are extensively found in the literature for different density functionals, such as the Shannon entropy [35] or frequency moments [34], but this is not the case for complexities, as they are constructed as a product of two different factors, that involves a lot of bounding procedure as compared to its application for single density functionals.

Here we are going to take advantage of the non-negativity of the so-called relative Fisher information between two functions. In what follows, and for the sake of simplicity, we will restrict ourselves to spherically symmetric densities, as is the case of atomic systems.

To do so, let us consider the non-negative integral

$$\int \rho(\mathbf{r}) \left(\frac{\mathrm{d}}{\mathrm{d}r} \ln \frac{\rho(r)}{f(r)}\right)^2 \mathrm{d}\mathbf{r} \geq 0 \tag{22}$$
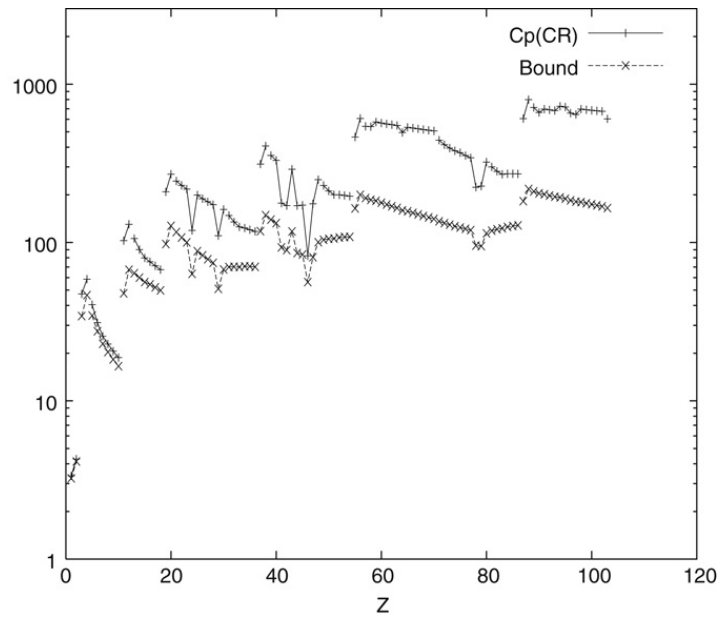
Fig. 3. Cramer–Rao complexity $C_p(CR)$ in momentum space, and lower bound in terms of radial expectation values, for neutral atoms with nuclear charge from $Z = 1$ to $Z = 103$. Atomic units (a.u.) are used.

where $f(r)$ is a (not necessarily normalized to unity) function, on which some conditions will be imposed below. By only carrying out the processes of derivation and squaring, and defining

$$F(r) \equiv \frac{f'(r)}{f(r)} \tag{23}$$

it is not difficult to find the relationship

$$\bar{I}_r \geq -\langle F^2(r)\rangle - 2\langle F'(r)\rangle - 2(n-1)\left\langle \frac{F(r)}{r}\right\rangle \tag{24}$$

where $\bar{I}_r$ refers to the Fisher information of the spherically averaged density $\rho(r)$, and the function $F(r)$ has to fulfill the condition $r^{n-1}\rho(r)F(r)\,|_0^\infty = 0$ for the finiteness of the expectation values.

So, for an appropriate choice of $F(r)$ the above expression provides a lower bound on the Fisher information in terms of expectation values of the density. Let us consider a choice of $F(r)$ for which the right-hand-side of Eq. (24) consists of a rational function in which the denominator is the variance $V_r = \langle r^2\rangle - \langle r\rangle^2$ and, consequently, the inequality transforms into a lower bound of the Cramer–Rao complexity $C_r(CR)$. Such a $F(r)$ is given by

$$F(r) = -\alpha\beta r^{\alpha-1} - \nu\gamma r^{\gamma-1}. \tag{25}$$

First, we optimize the resulting bound on the parameters (β, ν) and then we consider the particular case $(\alpha = 2, \gamma = 1)$, giving rise to

$$C_r(CR) \geq n^2 + (n-1)\langle r^{-1}\rangle\left[(n-1)\langle r^2\rangle\langle r^{-1}\rangle - 2n\langle r\rangle\right]. \tag{26}$$

Some comments are in order: (i) a similar bound for the corresponding quantity in conjugated space are obtained by considering the momentum density, and (ii) some radial moments (in both spaces) are specially relevant from a physical point of view. It is well known [42], for instance that, for many-electron systems, $\langle r^{-1}\rangle$ is essentially the electron-nucleus attraction energy, $\langle r^2\rangle$ is related to the diamagnetic susceptibility [42], $\langle p^{-1}\rangle$ is twice the height of the peak of the Compton profile [43], and $\langle p^2\rangle$ is twice the kinetic energy [43]. So, such a different quantities, physically relevant and/or experimentally accessible, provide also information on the Cramer–Rao complexity of the system.

In Fig. 3, a numerical computation of $C_p(CR)$ (momentum space) and the above mentioned particular bound (with $n = 3$ and momentum expectation values) is displayed for neutral atoms throughout the Periodic Table, with nuclear charge from $Z = 1$ to $Z = 103$. It is clearly observed the similar trends followed by the exact complexity and its lower bound. Both curves display a structure strongly related to the shell-filling process. A similar figure is obtained for the corresponding quantities in position space; therefore, the same comments as given above are also valid.

It is also worth mentioning that, contrary to the analyzed multi-electronic systems, none of the three complexities depends on the nuclear charge Z for one-electron systems (hydrogenic atoms), although the individual factors do (e.g. D_r

is proportional to Z^3 and I_r to Z^2, and inversely in conjugated space). In this sense, it is interesting to observe that such complexities can be analytically determined, their values being

$$C_r(LMC) = \frac{e^3}{8} = 2.5107 \tag{27}$$

$$C_r(FS) = \frac{2e}{\pi^{1/3}} = 3.712 \tag{28}$$

$$C_r(CR) = 3 \tag{29}$$

$$C_p(LMC) = \frac{66}{e^{10/3}} = 2.3545 \tag{30}$$

$$C_p(FS) = \frac{48(2\pi)^{1/3}}{e^{29/9}} = 3.5311 \tag{31}$$

$$C_p(CR) = 12\left(1 - \frac{64}{9\pi^2}\right) = 3.354. \tag{32}$$

As observed before, the multi-electronic character of the systems makes their complexities increase considerably compared to those of the corresponding one-electron ions.

4. Uncertainty-like complexity inequalities

It is natural to look for the existence of uncertainty-like relationships (i.e. involving the same density functionals simultaneously in both conjugated spaces) on the complexities considered in the present work. It appears very interesting to find rigorous and universal relationships among *conjugated complexities*, in a similar fashion to those verified, for instance, by the Shannon entropy (Bialynicki-Birula and Mycielski (BBM) lower bound $S_r + S_p \geq n(1 + \ln \pi)$ [44]), the variance (Heisenberg uncertainty principle [45]), the Fisher information [46] and the Renyi [47] and Tsallis [48] entropies. In all cases, the uncertainty inequality provides a constant lower bound (sometimes dependent on dimensionality) on the sum or product of the aforementioned conjugated information factors.

Apart from those inequalities on density functionals, there also exist uncertainty-like relationships between products of expectation values, as shown for instance in Ref. [49] for the radial ones.

So, in spite of the existing well-known uncertainty inequalities on most of the individual factors composing complexities, this is not the case (to the best of our knowledge) of the complexities themselves. The main reason is that, usually, the two inequalities associated with each factor work in opposite directions, making it impossible to combine them both in order to obtain a coherent bound on the whole complexity.

In this section, different uncertainty-like complexity inequalities are obtained, all with universal validity. This means that they hold for any pair of functions related via Fourier transform in the same way as the one-particle densities in the conjugated spaces do.

Let us also remark that, for the particular case of analyzing products of complexities $C_r \cdot C_p$, such a study is equivalent to considering the product or phase space complexity C_{rp}. However, the simple product operation of complexities is not at all the only way of getting uncertainty-like relationships, appearing also interesting to deal with quotients of complexities or of some of their powers, among others.

In this sense, it is worth mentioning that the ratio between the Fisher–Shannon and Cramer–Rao complexities on a given space can be bounded in terms of the so-called *uncertainty products*, expressed in terms, as mentioned above, of radial expectation values of both conjugated spaces. To do so, let us consider the ratio $C(FS)/C(CR)$ (in any space) which, attending to the definition of both complexities, turns out to be J/V in the same space. For simplicity, let us consider the position space ratio J_r/V_r, keeping in mind that all results obtained below will be also valid for the conjugated quantities. The BBM inequality between Shannon entropies can be written in terms of the power entropies as $J_r \cdot J_p \geq (\pi e)^{n-1}/2$, giving rise to a lower bound on the numerator J_r in terms of the power entropy J_p. On the other hand, upper bounds on the power entropy J_p in terms of any non-negative order radial expectation value $\langle p^\alpha \rangle$ are also well known [35]. Both inequalities together provide a lower bound on J_r in terms of $\langle p^\alpha \rangle$ with $\alpha > 0$.

Concerning the denominator V_r on the studied ratio, it is immediate from its definition that $1/V_r \geq 1/\langle r^2 \rangle$. Finally, combining both lower bounds results in the relationship

$$C_r(FS) \geq \frac{e^{1-\frac{2}{\alpha}}}{2}\left(\frac{n}{\alpha}\right)^{2/\alpha}\left(\frac{\alpha\,\Gamma(n/2)}{2\Gamma(n/\alpha)}\right)^{2/n}\frac{1}{\langle r^2\rangle\langle p^\alpha\rangle^{2/\alpha}}C_r(CR) \tag{33}$$

and similarly in the conjugated space by exchanging the involved variables. A numerical analysis of the above inequality is carried out (in position space) in Fig. 4 throughout the Periodic Table, for the particular case $\alpha = 1$. As in previous figures, we again observe the similar shape displayed by both the exact Fisher–Shannon complexity and its lower bound in terms of Cramer–Rao complexity and the chosen uncertainty product.
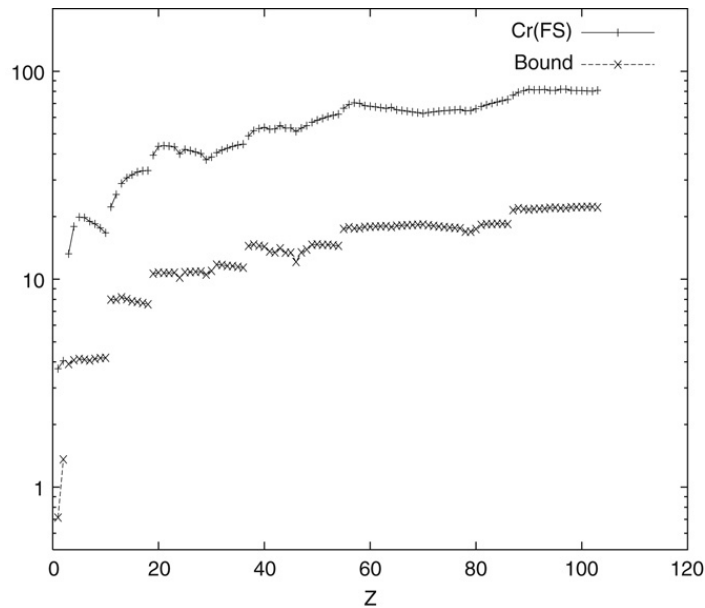
Fig. 4. Fisher–Shannon complexity $C_r(FS)$ in momentum space and lower bound in terms of Cramer–Rao complexity $C_r(CR)$, for neutral atoms with nuclear charge from $Z = 1$ to $Z = 103$. Atomic units (a.u.) are used.

Let us finally mention an uncertainty-like inequality on the LMC complexity product $C_r(LMC) \cdot C_p(LMC) = C_{rp}(LMC)$ in terms of arbitrary order uncertainty products of radial expectation values. In order to obtain it, let us remember that the factors appearing in the product space complexity consist of (i) the exponential entropy on rp-space, bounded from below by means of BBM inequality, and (ii) the disequilibriums (i.e. second-order frequency moments $D_r = \omega_r(2)$ and $D_p = \omega_p(2)$, as explained in Section 3), which are known both to be bounded from below in terms of two arbitrary radial expectation values of the associated density [34]. Choosing in both spaces as one radial constraint the normalization, the resulting bound on the uncertainty LMC complexity product results in

$$C_r(LMC) \cdot C_p(LMC) \geq e^n \Gamma^2(n/2)(n+\alpha)(n+\beta) \left(\frac{n}{n+2\alpha}\right)^{1+\frac{n}{\alpha}} \left(\frac{n}{n+2\beta}\right)^{1+\frac{n}{\beta}} \frac{1}{\langle r^\alpha \rangle^{n/\alpha} \langle p^\beta \rangle^{n/\beta}} \tag{34}$$

for radial expectation values orders $\alpha, \beta > -n/2$ in n-dimensional conjugated spaces. This result confirms the existence of a strong relationship between *complexity uncertainty* and uncertainty products in terms of radial expectation values. So, the knowledge of an uncertainty product imposes a constraint on the minimal value the LMC complexity product can reach.

5. Complexities of information-extremizer distributions

In this section, we obtain the values of complexities for extreme information distributions constrained by a given radial expectation value (apart from normalization). That is, let us consider the density $f(\mathbf{r})$ which maximizes or minimizes one of the previously studied information measures (e.g. the Shannon and Tsallis entropies, the Fisher information, the disequilibrium) among those normalized-to-unity functions with a given radial expectation value $\langle r^\alpha \rangle$. Such a density would be the solution of one of the so-called 'extremum information problems', which in general deal with an arbitrary set of constraints (neither necessarily one nor of radial type). However, for the present case there is a unique constraint, and most of the aforementioned methods provide an analytical solution, as shown in Ref. [50].

Let us focus on maximization of the Shannon S and Tsallis $T(q)$ entropies, and minimization of the Fisher information I [50]. The cited reference provides the analytical solution to the considered extremizations, for which the corresponding complexities are easily obtained, also analytically, for arbitrary order $\alpha > 0$ of the expectation value for the n-dimensional maximization problems, and for the particular case $\alpha = -1$ for the minimization three-dimensional case ($n = 3$). Let us denote complexities (whose expressions are exactly the same independently of the space considered) by using the subscript to specify the extremized functional (e.g. $C_S(LMC)$ refers to LMC complexity of the distribution which maximizes S, and similarly for the other complexities and extremized functionals). It is very remarkable that, although the individual factors of each complexity depends on the value of the constraint $\langle r^\alpha \rangle$, the complexity itself does not in any case. The obtained expressions are detailed below:

$$C_S(LMC) = (e/2)^{n/\alpha} \tag{35}$$

$$C_S(FS) = \frac{\alpha 2^{-\frac{2}{n}} \Gamma\left(\frac{n-2}{\alpha} + 2\right) e^{\frac{2}{\alpha} - 1} [2\Gamma(n/\alpha)]^{\frac{2}{n} - 1}}{\Gamma^{2/n}(n/2)} \tag{36}$$

$$C_S(CR) = \alpha^2 \frac{\Gamma\left(\frac{n-2}{\alpha}+2\right)}{\Gamma(n/\alpha)} \left[\frac{\Gamma\left(\frac{n+2}{\alpha}\right)}{\Gamma(n/\alpha)} - \left(\frac{\Gamma\left(\frac{n+1}{\alpha}\right)}{\Gamma(n/\alpha)} \right)^2 \right] \tag{37}$$

$$C_I(LMC) = e^{3/8} \tag{38}$$

$$C_I(FS) = \frac{2e}{\pi^{1/3}} \tag{39}$$

$$C_I(CR) = 3 \tag{40}$$

$$C_T(LMC) = \frac{B\left(\frac{n}{\alpha}, \frac{q+1}{q-1}\right)}{B\left(\frac{n}{\alpha}, \frac{q}{q-1}\right)} \exp\left\{ \frac{1}{q-1} \left[\Psi\left(\frac{q}{q-1} + \frac{n}{\alpha} \right) - \Psi\left(\frac{q}{q-1} \right) \right] \right\} \tag{41}$$

$$C_T(FS) = \frac{\alpha^{2-\frac{2}{n}}}{(q-1)^2 \Gamma^{2/n}(n/2)} \frac{B\left(2 + \frac{n-2}{\alpha}, \frac{2-q}{q-1}\right)}{\left[2B\left(\frac{n}{\alpha}, \frac{q}{q-1}\right)\right]^{1-\frac{2}{n}}} \exp\left\{ \frac{2}{n(q-1)} \left[\Psi\left(\frac{q}{q-1} + \frac{n}{\alpha} \right) - \Psi\left(\frac{q}{q-1} \right) \right] - 1 \right\} \tag{42}$$

$$C_T(CR) = \left(\frac{\alpha}{q-1} \right)^2 \frac{\Gamma\left(\frac{n}{\alpha} + \frac{q}{q-1}\right)}{\Gamma\left(\frac{n}{\alpha}\right)} \left[\frac{\Gamma\left(\frac{n+2}{\alpha}\right)}{\Gamma\left(\frac{n+2}{\alpha} + \frac{q}{q-1}\right)} - \frac{\Gamma^2\left(\frac{n+1}{\alpha}\right) \Gamma\left(\frac{n}{\alpha} + \frac{q}{q-1}\right)}{\Gamma^2\left(\frac{n+1}{\alpha} + \frac{q}{q-1}\right) \Gamma\left(\frac{n}{\alpha}\right)} \right] \tag{43}$$

where $B(x, y)$ denotes the *beta function* and $\Psi(x) = \frac{\Gamma'(x)}{\Gamma(x)}$ the *digamma function*; last two equations are valid only for the range $1 < q < 2$, because those two complexities contain the Fisher information I of the maximum Tsallis entropy distribution, which integral only converges within such a range. Let us observe, however, that maximization of the Tsallis entropy $T(q = 2)$ is equivalent to minimization of the disequilibrium (i.e. second-order frequency moment) D. So, the corresponding LMC complexity (the only one well defined in this case) of minimum disequilibrium distribution is

$$C_D(LMC) = \frac{2\alpha}{2\alpha + n} \exp\left\{ \Psi\left(2 + \frac{n}{\alpha} \right) - \Psi(2) \right\} \tag{44}$$

which corresponds to the particular value $q = 2$ in Eq. (41).

Some comments are in order: (i) as previously mentioned, it is observed that the final expressions for analytical complexities do not depend on the constraint value $\langle r^\alpha \rangle$, but only on its order; (ii) we are still left with the problem of finding the *maximum/minimum complexity distribution* under such constraints; that is, it is not guaranteed that the distribution that maximizes (minimizes) one factor of complexity be the same that also extremizes the whole complexity; and (iii) it would also be possible to consider a higher number of constraints, but in such a case the extremizer distribution (i.e. the solution to the associated variational problem) would not be analytically obtained and, consequently, the same would happen with complexity, for which the Lagrange multipliers should be numerically determined.

6. Conclusions

Complexity measures are useful quantities to interpret different structural properties of systems or processes. Attending to the main complexity definitions in terms of the Shannon entropy, the Fisher information and the variance, several rigorous properties have been shown. Such properties include universal bounds, limiting expressions, relationships among themselves and/or radial expectation values and uncertainty products, as well as the exact values for specific functions (e.g. hydrogenic densities and information-extremizer distributions). All results obtained in here are valid for arbitrary systems, and were numerically tested in atomic systems for the sake of completeness.

Acknowledgments

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