Atomic complexity measures in position and momentum spaces

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Fisher–Shannon (FS) and López-Ruiz, Mancini, and Calbet (LMC) complexity measures, detecting not only randomness but also structure, are computed by using near Hartree–Fock wave functions for neutral atoms with nuclear charge $Z=1-103$ in position, momentum, and product spaces. It is shown that FS and LMC complexities are qualitatively and numerically equivalent for these systems. New complexity candidates are defined, computed, and compared by using the following information-theoretic magnitudes: Shannon entropy, Fisher information, disequilibrium, and variance. Localization-delocalization planes are constructed for each complexity measure, where the subshell pattern of the periodic table is clearly shown. The complementary use of r and p spaces provides a compact and more complete understanding of the information content of these planes. © *2008 American Institute of Physics*. [DOI: 10.1063/1.2907743]

I. INTRODUCTION

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] Fisher information,[4,5] logical depth,[6] thermodynamical depth,[7] computational mechanics,[8] and others. Most share formal similarities with the others as well as with Bayes and information theory.[9]

Indeed, the term complexity has many different meanings and adjectives (algorithmic, geometrical, computational, stochastic, effective, statistical, and structural) and is used in very diverse fields (dynamical systems, time series, quantum wave functions in disordered systems, spatial patterns, language, analysis of multielectronic systems, cellular automata, neuronal networks, self-organization, molecular or DNA analyses, social sciences, etc.).[10–12] 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 last years.[13,14]

Therefore, the characterization of complexity cannot be univoque and must be adequate to the type of structure or process we study, to the nature and goal of the description we want, and to 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 capture not only uncertainty or randomness can be searched. One wishes also to capture some other properties distinct from randomness, such as clustering, order, or organization of a system or process. Some of the definitions and relations between the above concepts are not clear and even less how disorder or randomness take part in the aforementioned properties of the system and vice versa.

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. This is the case of the characterization of López-Ruiz, Mancini, and Calbet complexity[15] C(LMC) that, like others, satisfies the boundary conditions of vanishing in the extreme ordered and disordered limits. The LMC complexity measure C(LMC) has been criticized,[13,16] modified[17,18] and generalized,[19,20] leading to a useful estimator which satisfies several desirable properties of invariance under scaling, translation, and replication. The utility of this improved complexity has been checked in many fields[11,12,20] and allows reliable detection of periodic, quasiperiodic, linear stochastic, and chaotic dynamics.[15,20,21] Another simple and related measure of complexity has been also proposed by Shiner, Davison, and Landsberg (SDL complexity) as a product of disorder-order factors.[18,22]

The LMC measure, $C(\mathrm{LMC}) \equiv De^{S}=DL$, is constructed as the product of two important information-theoretic quantities: The so-called disequilibrium D (also known as self-similarity[23] and information energy[24]), which quantifies the departure of the probability density from uniformity,[15] and the Shannon entropy S, which is a general measure of randomness or uncertainty of the probability density.[3] Both global magnitudes that play an important role in information theory are closely related to measures of spread of a probability density, such as the variance V (which measures the spreading of the density from its mean value), and are called

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Renyi lengths ($L=e^S$ and $1/D$) in other contexts.[25] Renyi entropies are just the logarithm of these spread measures.[26]

Some uncertaintylike relations between the above information magnitudes are known, establishing connections between position r and momentum p spaces. For instance, the well known Heisenberg inequality, $V_r V_p \geqslant n^2/4$,[27] with n being the space dimensionality, the more stringent relation $S_r + S_p \geqslant n(1+\ln \pi)$,[28] and the lower bound to the Fisher information product, $I_r I_p \geqslant 4n^2$ [Refs. 29 and 30] for central potentials (conjectured to be also valid in the general case).

We will concentrate in the application of LMC-type complexity measures to the study of multielectronic systems and, in particular, to neutral atoms, where the one-particle density, in position and momentum spaces, is the fundamental magnitude in this kind of studies.

Very recently, a new candidate for measuring the information content of atomic systems was presented as the product of Fisher information (I) and power Shannon entropy $J \equiv (1/2\pi e)L^{2/3}$.[31] In this form, a local magnitude I, which measures the gradient content of the probability distribution, is used instead of the disequilibrium D to quantify the level of organization and pattern of the corresponding system. We call this new measure, $C(\mathrm{FS}) \equiv IJ$, the Fisher–Shannon complexity. Factors in the "power Shannon entropy" J are chosen to have the rigorous uncertainty relationship $C(\mathrm{FS}) = IJ \geqslant n$.[32]

The well known Cramer–Rao bound $IV \geqslant 1$ (for dimension $n=1$ and infinite support interval)[32,33] relates also two important information measures, i.e., Fisher information and variance, and will lead us to study a complexity measure defined in terms of these magnitudes.

The aim of this work is to carry out a complete analysis of information-theoretic and complexity measures for atomic systems with nuclear charge $Z=1-103$, studying uncertainty, localization, structure, and information content of these simple but strongly structured systems.

To do this, in Sec. II, we use the above information measures, L, D, I, V, and J, to compute Fisher–Shannon and LMC complexity measures. We study all the information magnitudes in the position and momentum spaces, as well as in a joint product space rp that contains all the information about the system. Fisher–Shannon and disequilibrium-Shannon planes show the complementary behavior of the complete set of atoms in the conjugated spaces, and the shell-filling pattern throughout the periodic table of elements. In Sec. III, new proposals of complexity estimators are defined, computed, and compared to the previous ones. Results and conclusions are remarked in the last section.

II. LMC AND FS COMPLEXITY MEASURES IN ATOMIC SYSTEMS

In this section, the strong correlation between the "complexity" concepts (as previously defined in terms of different global and local properties of the distribution) and some relevant chemical and physical properties of atomic systems (e.g., nuclear charge, shell-filling) is deeply analyzed by means of their one particle densities in the three-dimensional ($n=3$) position and momentum spaces, $\rho(\mathbf{r})$ and $\gamma(\mathbf{p})$, respectively, which are well known to play a relevant role in the description of many fermion systems.

The entropic quantities defined in the general case are now expressed, in terms of the normalized-to-unity one-particle densities, as follows: Shannon entropy

$$S_r = -\int \rho(\mathbf{r}) \ln \rho(\mathbf{r}) d\mathbf{r}, \tag{1}$$

from which exponential entropy $L_r = e^{S_r}$ and power entropy $J_r = e^{2/3 S_r}/2\pi e$ are also defined, disequilibrium

$$D_r = \int \rho^2(\mathbf{r}) d\mathbf{r}, \tag{2}$$

Fisher information

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

and variance

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

with $\langle r^k \rangle \equiv \int r^k \rho(\mathbf{r}) d\mathbf{r}$ the radial expectation values of the distribution. According to these definitions, the corresponding complexity measures $C_r(\mathrm{LMC})$ and $C_r(\mathrm{FS})$ are built up.

All the above expressions correspond to the position space density $\rho(\mathbf{r})$. Similar definitions are also valid in momentum space by only replacing the density $\rho(\mathbf{r})$ by $\gamma(\mathbf{p})$ as well as the associated independent variable. In what follows, we will employ the subscripts r or p according to the space and density we are dealing with. For the present case (i.e., neutral atoms), it is sufficient to consider the spherically averaged densities $\rho(r)$ and $\gamma(p)$ for a full description of the system.

Other authors have recently dealt with some particular factors of the complexity measures. In particular, Shannon entropy has been extensively used in the study of many important properties of multielectronic systems, such as, for instance, rigorous bounds,[34] electronic correlation,[35] effective potentials,[36] similarity,[37] and minimum cross entropy approximations.[38]

More recently, Fisher information has been studied as an intrinsic accuracy measure for concrete atomic models and densities[39,40] and also for quantum mechanics central potentials.[41] Also, the concept of phase space Fisher information, where position and momentum variables are included, was analyzed for hydrogenlike atoms and the isotropic harmonic oscillator.[42] Quantum similarities and self-similarities (D) for neutral atoms were computed for $Z=1-54$ only in the position space,[43,44] but afterwards a more complete analysis including $Z=1-103$ neutral systems and singly charged ions has been done in position and momentum spaces.[45]

Complexity studies for atoms have also been carried out, but most of them are only for $Z=1-54$.[12,46] Recent complexity computations, using relativistic wave functions in the position space, were also done.[47] Some other complexity works simply take the position density,[48] not the momentum one as basic variable. In this sense, it is worthy to point out the

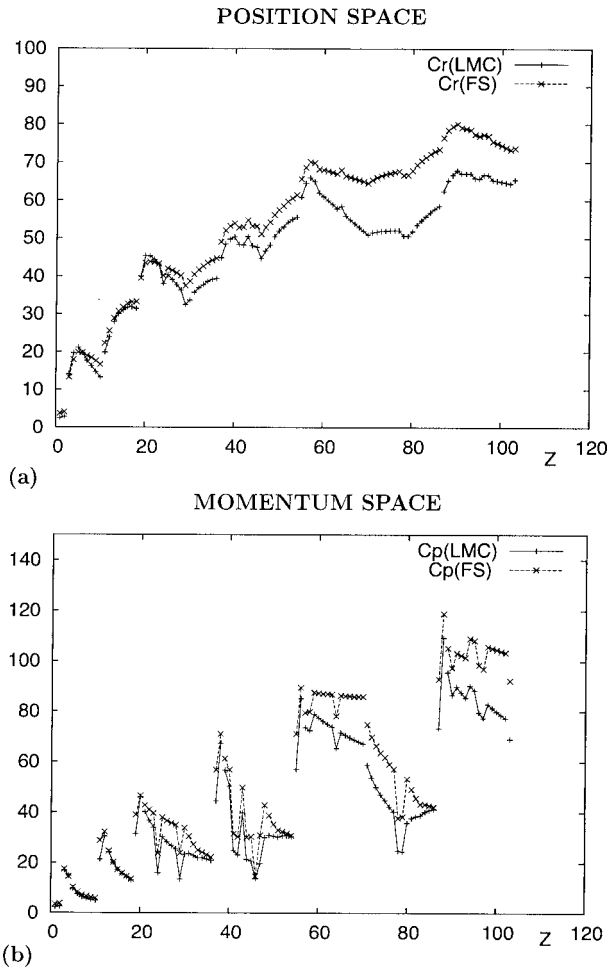

FIG. 1. $C(\mathrm{LMC})=DL$ and $C(\mathrm{FS})=IJ$ complexities for neutral atoms with nuclear charge $Z=1-103$ in (a) position space and (b) momentum space. Atomic units (a.u.) are used.

different behaviors displayed by some of these quantities in position and momentum spaces for atomic systems, as we have recently shown.[49,50]

For carrying out the numerical calculations needed in order to analyze the aforementioned quantities in atomic systems, as well as the relationships among themselves, we have employed the accurate near-Hartree–Fock wave functions of Koga *et al.*,[51] which provide the one-particle densities $\rho(\mathbf{r})$ and $\gamma(\mathbf{p})$ for neutral atoms with nuclear charge within the range of $Z=1-103$, from which the entropic and informational quantities are computed.

The first step in the present complexity-based study is to analyze the different information provided by the LMC and FS complexities for the whole set of atomic system considered here. A comparison between both complexities can be established attending to the results displayed in Fig. 1, where they are plotted as a function of the nuclear charge Z in each conjugated space, namely, position [Fig. 1(a)] and momentum [Fig. 1(b)]. In both cases, the strong structural similarity between the C(LMC) and C(FS) clearly appears. Here, let us remark that each complexity consists of two factors, one of them always defined in terms of the Shannon entropy S, being the other factor that characterizes more specifically the corresponding complexity because we are using a *global* quantity (i.e., disequilibrium D) for C(LMC) and a *local* one (i.e., Fisher information) for C(FS). Nevertheless, there are no relevant structural differences between complexities based on the global or the local one. Additionally, such a comment can be done independent of the conjugate space considered.

Another relevant characteristics of all curves plotted in Figs. 1(a) and 1(b) are (i) the similar magnitude order of both complexities, taking into account their different definitions and (ii) the strong correlation appearing between the shell-filling process in atomic systems (and also the group which atom belongs to) and location of extrema (maxima and minima) or, equivalently, monotonicity (increasing or decreasing) between consecutive extrema.

It is worthy to point out that, with very a few exceptions, C(LMC) and C(FS) in both position and momentum spaces reach minimum complexity values for noble gases as well as for the *anomalous shell-filling* set of atoms (specially remarkable are the values $Z=24,29,46$, all characterized for *losing* an s electron). Also maxima are frequently associated with shell structure. Nevertheless, in order to associate their location with the shell-filling process, it is better to do it separately for position and momentum spaces. In this sense, it is remarkable the fact that, with only two exceptions in momentum space (namely, subshells $5p$ and $6p$), the monotonic behavior of both LMC and FS in position and momentum spaces are exactly the same. Taking this fact into account, we will discuss such a behavior referring only to complexity having in mind that discussion is applicable to any of them.

As mentioned above, both complexities display exactly the same monotonic behavior within each subshell in position space. These comments allow us to assure that, for instance, complexity always increase in position space when adding s electrons. Last comment can also be done for momentum space complexity (with the only exception of $Z=4$). However, monotonic behavior for non-s subshells is opposite to that of position space.

So, the connection between shell-filling patterns and complexity values is very clearly stated. Let us remark again that complexity is composed of two factors. In this sense, it is also interesting to analyze the contribution of each one to the total complexity which, for the present purposes and as a consequence on comments of Fig. 1, essentially reduces to the study of Shannon entropy (by means of the exponential entropy L) and disequilibrium D. This is done in Fig. 2, where such a *disequilibrium-Shannon plane* is shown in both position [Fig. 2(a)] and momentum [Fig. 2(b)] spaces. Again, the shell-filling patterns are observed in both cases, much more clearly in momentum than in position space, requiring, in this last case, a detailed analysis of location of extrema and monotonic behaviors. Nevertheless, two important points should be pointed out concerning the differences of both position and momentum planes: (i) Pieces of curve in momentum spaces belong to independent and disjoint *ranges of values* in ordinate axis (i.e., exponential entropy L_p), increasing when involving a new outer subshell, while disequilibrium D_p shows a decreasing trend when adding electrons within an specific subshell; however, position space quanti-

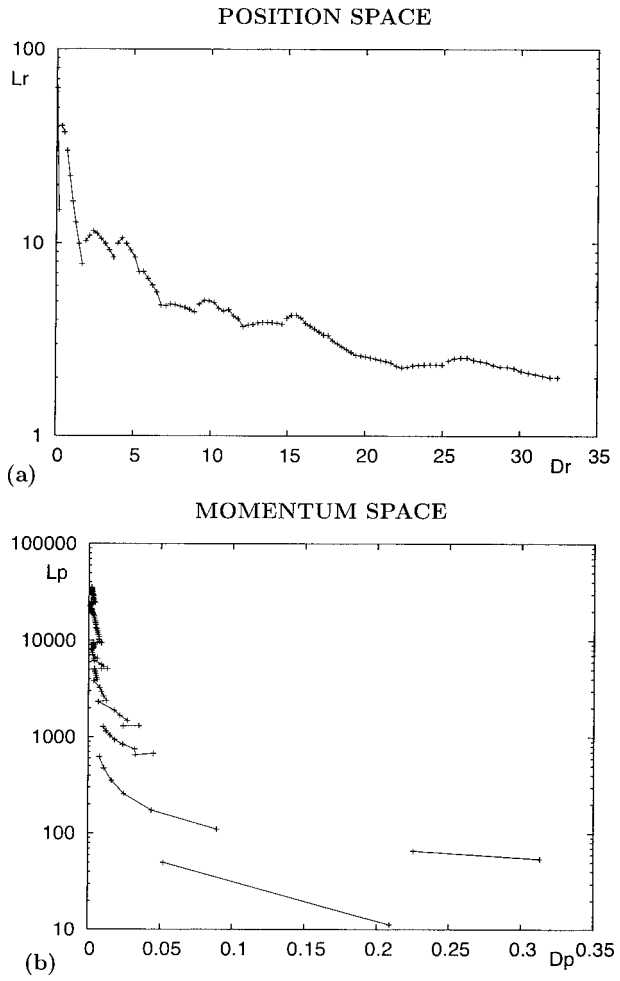

FIG. 2. Disequilibrium-Shannon plane (D,L) for neutral atoms with nuclear charge $Z=1-103$ in (a) position space and (b) momentum space. Atomic units (a.u.) are used.

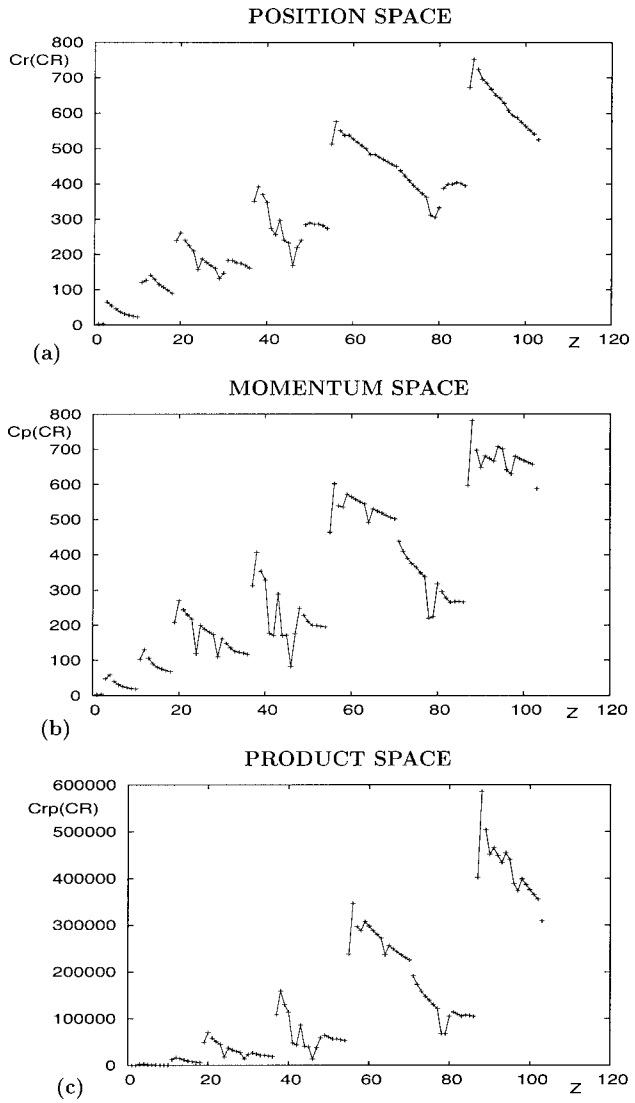

FIG. 3. $C(\mathrm{CR})=IV$ complexity for neutral atoms with nuclear charge $Z=1-103$ in (a) position space, (b) momentum space, and (c) product space. Atomic units (a.u.) are used.

ties L_r and D_r display exactly the opposite monotonic behaviors; (ii) the aforementioned trends for all the involved quantities defining both planes make the heavy atoms to *concentrate* at different locations attending to the space we are dealing with, namely, on the lower-right corner (position space) and the upper-left one (momentum space).

III. CRAMER–RAO INFORMATION PLANE AND OTHER COMPLEXITY MEASURES

Taking those previously mentioned factors as basic information, additional quantifications of complexity for different systems and processes should also be considered. In this sense, the so-called *Cramer–Rao* product has been considered in other contexts.[52] It is defined as $C(\mathrm{CR})\equiv IV$, i.e., in terms of two very different (attending to their definitions) factors, again a local (I) and a global (V) one.

Nevertheless, the existence of a nontrivial lower bound for a product of information factors,[32,33] which such a very different origin and definition in terms of the density, reveals again the strong relation connecting the *degree of uncertainty* in both the local and global sense.

Concerning the behavior of the Cramer–Rao complexity $C(\mathrm{CR})$ throughout the periodic table, in a similar way as done in Sec. II for $C(\mathrm{LMC})$ and $C(\mathrm{FS})$ complexities, its dependence on the nuclear charge Z and correlation with atomic shell structure are clearly displayed in Fig. 3 in the three spaces r, p, and rp.

It is firstly observed that many of the minima of $C_r(\mathrm{CR})$ and all of them for $C_p(\mathrm{CR})$ also appeared in both complexities discussed in the previous section. Moreover, shell structure patterns are almost identical for the three complexities, where up to five different factors (exponential entropy, disequilibrium, power entropy, Fisher information, and variance) have been employed.

In order to justify some of those similarities among complexities, it appears interesting to compare the different individual factors mentioned above. An example is shown in Fig. 4, where a comparison between the exponential entropy L (a factor in LMC complexity) and the variance V (within the Cramer–Rao complexity) is carried out in both conjugated spaces. Again, a strong structural similarity between both quantities of such a different origin, in a different way in each space can be clearly observed. In position space, again, local minima are almost identically localized in both

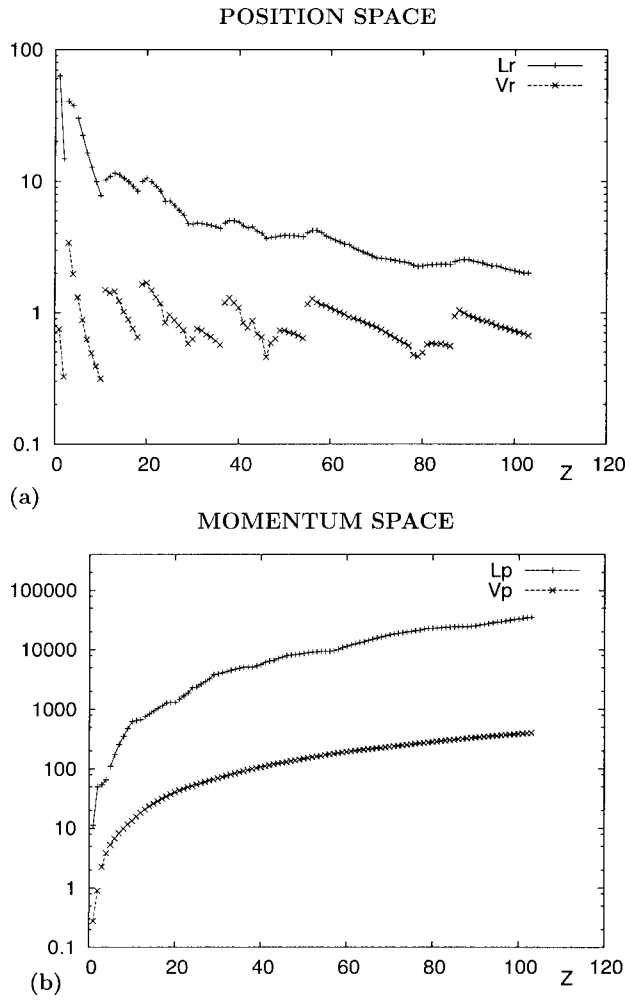

FIG. 4. Exponential entropy (L) and variance (V) for neutral atoms with nuclear charge $Z=1-103$ in (a) position space and (b) momentum space. Atomic units (a.u.) are used.

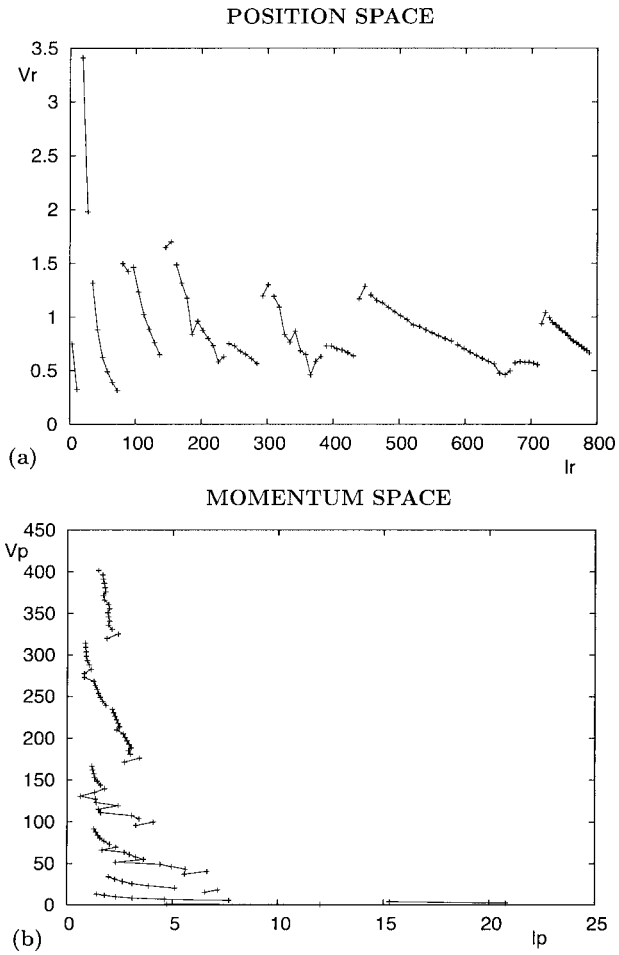

FIG. 5. Cramer–Rao plane (I,V) for neutral atoms with nuclear charge $Z=1-103$ in (a) position space and (b) momentum space. Atomic units (a.u.) are used.

curves, which are composed of *monotonic pieces* associated with shell-filling, as discussed in the previous figures. However, such shell-filling pattern is much more clearly observed in the variance than in the exponential entropy.

On the other hand, similarity in momentum space consists of a monotonically increasing behavior for both quantities when increasing the nuclear charge, showing an almost identical shape differing only by a scaling factor.

It is important to note here, looking at Figs. 1, 3, and 4, how complexity measures detect not only randomness or disorder but also the own structure and organization of the physical systems that we are dealing with. Indeed, Fig. 4(a) shows two measures of spread (V_r) and randomness (L_r), which are both peaked and decreasing in r space, showing that the uncertainty related to heavy systems is smaller than the one corresponding to light atoms. Nevertheless, for large Z, the exponential entropy L_r is a rather monotone function of Z. In a similar way, localization (D_r) or accuracy factors (I_r) are strictly monotonic increasing functions of Z in position space. However, the corresponding LMC or CR complexities, in position space (plotted in Figs. 1 and 3, respectively) show very different increasing and rugged behavior.

This different trend of entropy and complexity is even more clear in momentum space, where exponential entropy (L_p) and variance (V_p) are smooth monotonic increasing functions [see Fig. 4(b)] whereas respective complexities are peaked and structured functions of Z, showing all the complex organization of the atomic shell structure. Localizations (D_p or I_p) in this space are the factors which incorporate structure to the complexity measures. Therefore, the utilization of localization and randomness factors to construct complexities, as well as the complementary use of position and momentum spaces are fundamental to having a complete description of the information content of the atomic systems. In this sense, Fig. 3(c), which shows the Cramer–Rao complexity in the product space, is a good example of the completely structured behavior of the periodic table of elements.

One could also wonder, concerning the connection between location of extrema and shell structure in both spaces, if such a connection is mainly due to one specific factor of Cramer–Rao complexity or, perhaps, to both of them. This is the main purpose of Fig. 5, in which the Cramer–Rao plane is drawn in both spaces for the atomic systems considered here. Keeping in mind that shell structure was previously well displayed in both conjugate spaces, the different origins of the local extrema when dealing with position and momentum space are non observed. In this sense, Fig. 5(a) (position space) reveals that in going from one subshell to the next

one, Fisher information I_r appreciably increases its value; in fact, ranges of values of I_r for each specific subshell are represented as a disjoint set of intervals over the abscissa axis. However, the same is not true for the variance V_r where a monotonically decreasing behavior is displayed within each individual subshell (apart from the aforementioned anomalous shell-filling exceptions), but now with most of the corresponding associated ranges overlapped within a narrow interval of values. Additionally, the increasing tendency of I_r and the decreasing of V_r against Z make the heavy atoms to appear *concentrated* next to the lower-right corner of the figure.

A similar analysis to that given above, but now in momentum space [Fig. 5(b)], provide an exactly opposite behavior concerning V_p and I_p factors. Now, it is the variance, the factor, which displays such a *subrange of values* decomposition (i.e., increasing variance when considering an outer valence subshell atom), while the decreasing behavior with a subshell is now associated with Fisher information I_p. Both opposite monotonic behaviors compare to those of position space make now the heavy atoms to appear next to the upper-left corner.

The above discussion establishes again a common property to the previously analyzed disequilibrium-Shannon plane (Sec. II), where similar trends concerning shell structure and location of light and heavy atoms were observed.

Finally, we have also analyzed other possible complexity measures based on the individual information factors considered here, such as the products obtained when replacing the factor on the Cramer–Rao complexity by a complementary one (also in all spaces). For instance, the products DV (where disequilibrium replaces Fisher information) and IL (with variance replaced by exponential entropy). For the sake of simplicity, we do not show here the associated figures, but a detailed study of both local extrema and range of values of individual factors provide similar conclusions to those deeply analyzed for other complexities.

IV. CONCLUSIONS

We have used some information-theoretic magnitudes, measuring randomness (S,L,J), spread (V), localization (D), and intrinsic accuracy (I) to compute several measures of complexity, each one consisting of two localization-delocalization factors: $C(\mathrm{LMC})=DL$, $C(\mathrm{FS})=IV$, $C(\mathrm{CR})=IV$, and the products DV and IL. We have tested these proposals on atoms, known to be strongly organized and hierarchical systems.

It is observed 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 behavior of these systems. The universality of the method allows one to apply it to any multifermionic system by using the corresponding one-particle density in both conjugated spaces.

We have shown that LMC and Fisher–Shannon complexity measures (using respectively very different, global and local, first localization factors) give similar qualitative and quantitative results for neutral atoms for $Z=1-103$ in both position and momentum spaces. This result contrasts with other previous ones, where diverse atomic information magnitudes must be arbitrarily factorized or scaled in order to compare them.

The pattern of the periodic table is clearly displayed, and the shell-filling process is readily captured by the measures. Atoms are clustered according to their atomic groups and a similar structure within each atomic period is found. Position and momentum analyses provide a complementary display of this structure. In general, position space patterns in localization-delocalization planes are inverse, as one would expect according to the uncertainty relations, to those of momentum space.

New proposals of LMC-type complexity measures (*IV*, *DL*, and *IL*) are constructed and computed for the whole set of physical systems. In particular, we concrete in the Cramer–Rao complexity (*IV*) where the external global character of S is changed by another well known spread measure (now centered on the average position): The variance V. We conclude that similar trends are followed by this measure, capturing faithfully not only randomness or localization but also the rich organization of the periodic table in the complementary conjugated spaces.

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