
Complexity Analysis of Ionization Processes and Isoelectronic Series

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ABSTRACT: Information-theoretic magnitudes measuring randomness (Shannon entropy, exponential entropy, power entropy), spread (variance), localization (disequilibrium or self-similarity) and intrinsic accuracy (Fisher information) are used to compute several measures of complexity consisting, each one, of two localization–delocalization factors. These proposals have been tested on known, simple, but strongly organized and hierarchical systems (atoms) and processes (ionization). A complete numerical analysis at the Hartree–Fock level is done in position, momentum, and product spaces, where similar trends are followed by all studied complexities. It is also found that the complexity planes clearly reveal shell-filling patterns across the periodic table. Characteristic features accompanying the ionization process are identified, and the physical reasons for the observed patterns are described. We conclude that (i) the studied complexity measures detect not only randomness or localization, but also pattern and organization, and (ii) their study is not only sufficient in the usual position space, but also in the complementary momentum space, to have a complete description of the information–theoretic behavior of these systems. © 2008 Wiley Periodicals, Inc. *Int J Quantum Chem* 109: 586–593, 2009

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1. Introduction

Measuring the complexity of a general system is an important area of contemporary research, which has roots in Information and Bayesian theories [1, 2]. Till the present date, different definitions of the complexity have been proposed. Among these, a few notable definitions include algorithmic or Kolmogorov–Chaitin complexity [3, 4], Lempel–Ziv complexity [5], effective measure of complexity by Grassberger [6], logical depth by Bennett [7], and thermodynamical depth by Lloyd and Pagels [8].

In most of the proposals for complexity measures, employment of the concept of entropy or relevant information can be regarded as a basic ingredient for quantifying the phenomenon. In the last few years, keen interest in developing new definitions for statistical measure of complexity based on probabilistic descriptions of physical systems has emerged. One of them is the disequilibrium-based complexity, denoted by LMC because of its pioneering authors López-Ruiz, Mancini and Calbet, which is defined as $C = D \cdot S$ [9], where S is the Shannon entropy and D the so-called disequilibrium that has adopted quadratic distances of each state for assessing the equiprobability [10]. This later important magnitude has been also named self-similarity [10], Onicescu information energy, [11] or principal number [12], in other contexts. The other measure of complexity is the simple one proposed by Shiner et al. [13]. It is defined as the product of a measure of order and a measure of disorder in a system, and it is related to LMC complexity.

The LMC complexity has been criticized [14] and modified [15], leading to a measure $C(\text{LMC}) = D \cdot L = D \cdot e^S$ [16], which satisfies several desirable properties of invariance under scaling, translation, and replication and has been further generalized [17] to include Renyi and Tsallis entropy measures. Both global factors of $C(\text{LMC})$ play an important role in Information Theory, are closely related to measures of spread of a probability density, like the variance V (which measures the spreading of the density from its mean value), and are called Renyi lengths ($L = e^S$ and $1/D$) in other contexts [18]. Renyi entropies are just the logarithm of these two spread measures [19]. The utility of such generalized complexity measures has been demonstrated recently [20–22].

More recently Fisher–Shannon complexity $C(\text{FS}) = I \cdot J$ [23] was presented and tested in atomic systems, having the advantage of using a local magnitude to measure intrinsic accuracy, the Fisher information I , and a global magnitude to quantify randomness, i.e. the power entropy $J = e^{(2/n)^S} / (2\pi e)$, where n is the dimension of the space.

Information–theoretic properties have been used in recent years for the study of quantum mechanical and multielectronic systems. In particular, their use in atomic and molecular physics has led to a new insight in these fields [24–27].

In the present work we carry out a systematic study of the following information–theoretic magnitudes: Fisher information (I) or disequilibrium (D) to measure intrinsic accuracy or localization respectively, and exponential Shannon entropy ($L = e^S$) or variance (V) to measure uncertainty or delocalization. New complexity candidates are defined, computed, and compared using these two localization–delocalization factors and leading to complexity measures of order–disorder type: $C(\text{LMC}) = D \cdot L$, Cramer-Rao complexity $C(\text{CR}) = I \cdot V$ and also the other two possibilities: $D \cdot V$ and $I \cdot L$, besides the previously used Fisher–Shannon complexity $C(\text{FS})$.

In this work these LMC-type complexities are tested on simple, but strongly organized N -electronic systems, $N = 1$ –54, of neutral atoms and their singly charged ions. In Section 2 we define and present the main properties of the magnitudes we are dealing with. In Section 3 the behavior in the localization–delocalization planes accompanying the process of gain or loss of one electron for an atom at constant nuclear charge Z is studied. In Section 4 the isoelectronic variation of this information measures of over a fairly extended range of Z values is presented. Both partial variations with respect to the electron number N and the nuclear charge Z are found to show characteristic features in the complexity planes. The complementary use of \mathbf{r} and \mathbf{p} spaces provides a compact and more complete understanding of the information content of these planes. Conclusions and main results are collected in the last section.

2. LMC-Type Complexities in Atomic Systems

The information theoretic magnitudes presented in the introduction are now defined and expressed in terms of the one particle densities in the three dimensional ($n = 3$) conjugated position and mo-

mentum 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. Concerning the normalized to unity one-particle density in position space, Shannon entropy is given by

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

from which exponential and power entropies, $L_r = e^{S_r}$ and $J_r = e^{2/3S_r}/2\pi e$ respectively, are consequently obtained; also disequilibrium

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

Fisher information

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

and variance

$$V_r = \langle r^2 \rangle - \langle r \rangle^2 \quad (4)$$

(with $\langle r^k \rangle = \int r^k \rho(\mathbf{r}) d\mathbf{r}$ being radial expectation values) are the corresponding quantities for the distribution $\rho(\mathbf{r})$. Similar definitions are considered for the momentum density, where the subscript r is replaced by p , as well as for the joint product space where the aforementioned quantities will be denoted with the subscript rp . This space shows, in a very compact form, all the information content of the process or system we are dealing with and leads to a more complete understanding of the total behavior of complexity, taking into account the information coming from both conjugated spaces. The information magnitudes in product space are defined as the product of the corresponding ones for each isolated space, with the only exception of power entropy J_{rp} in which the denominator $2\pi e$ appears only once. Notice that for some of those quantities, the aforementioned products are also the result of evaluating the same magnitudes for the product distribution function $f(\mathbf{r}, \mathbf{p}) = \rho(\mathbf{r})\gamma(\mathbf{p})$.

In what follows, we will only deal with the spherically averaged densities $\rho(\mathbf{r})$ and $\gamma(\mathbf{p})$, being sufficient for a complete description of the distributions analyzed in the present work, namely those corresponding to atomic systems.

According to these definitions, the corresponding complexity measures in position space $C_r(\text{LMC}) = D_r \cdot L_r$, $C_r(\text{CR}) = I_r \cdot V_r$, $C_r(\text{DV}) = D_r \cdot V_r$, and $C_r(\text{IL}) = I_r \cdot L_r$ are built up, in addition to $C_r(\text{FS}) = I_r \cdot J_r$, and similarly in the other two spaces.

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 [28], electronic correlation [26], effective potentials [29], similarity [30, 31], electric and magnetic fields [32], local properties [33], and maximum entropy approximations [34].

More recently, Fisher information has been studied as an intrinsic accuracy measure for concrete atomic models and densities [35, 36] and also for quantum mechanics central potentials [37]. Quantum similarities and self-similarities (D) for neutral atoms were computed for $Z = 1-54$ only in the position space [38, 39] but afterwards a more complete analysis including $Z = 1-103$ neutral systems and several singly charged ions has been done not only in position but also in momentum space [40].

Complexity studies for neutral systems have also been carried out, but most of them only for $Z = 1-54$ [41]. Some others complexity works simply take as basic variable the position density [42, 43], but not the momentum one. In this sense, it is worthy to point out the different behavior displayed by some of these quantities for atomic systems attending to the considered space, as we have recently shown [44, 45].

Some uncertainty-like relations between the above information magnitudes are known, establishing connections between position, r , and momentum, p , spaces. For instance the well-known n -dimensional Heisenberg inequality, $V_r \cdot V_p \geq n^2/4$ [46], the more stringent relation $S_r + S_p \geq n(1 + \ln \pi)$ [47], and the lower bound to the Fisher information product $I_r \cdot I_p \geq 4n^2$ [37, 48] for central potentials (conjectured to be also valid in the general case).

The previously introduced informational measure $C(\text{FS}) = I \cdot J$ takes into account global (J) and local (I) characteristics of the electronic densities. Besides, one factor (J) measures randomness or uncertainty whereas the other one measures localization or intrinsic accuracy (I) in the corresponding electronic system. This product informational measure has been recently proposed as a new candidate for measuring complexity/organization of systems

and processes in a similar form than SDL or LMC complexities do [23].

Factors in the Shannon-based power entropy J are chosen for the rigorous uncertainty relationship $C(\text{FS}) = I \cdot J \geq n$ to be verified [49]. The well-known Cramer-Rao bound $I \cdot V \geq 1$ (for dimension $n = 1$ and infinite support interval)[49, 50] also relates two important information measures, i.e. Fisher information and variance, leading us to study a complexity measure defined as the product of these magnitudes.

In the following sections 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, (as well as in product space), properties which are well-known to play a relevant role in the description of many fermion systems.

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 wavefunctions of Koga et al. [51, 52], which provide the one-particle densities $\rho(\mathbf{r})$ and $\gamma(\mathbf{p})$ for neutral atoms, anions, and cations with not more than $N = 54$ electrons, and isoelectronic series with $N = 2-10$ and nuclear charge within the range $N \leq Z \leq N + 20$, for which the entropic and informational quantities are computed.

In particular, we compute all the above mentioned complexities in each conjugated (r and p) and product (rp) spaces, for those systems. Therefore, we can study, on the one hand, the effect of complexities of loosing or gaining valence electrons and, on the other, the effect that the size of the nucleus has in these complex electronic systems.

Extensive computations lead to rather similar qualitative results for all LMC-type complexity measures we have dealt with. We will center our attention in Section 3 in the study of the complexity trajectories followed in monoionization processes, showing first that LMC and FS complexity give very similar numerical results. Then the ionization processes are analyzed, for variety, using the Cramer-Rao complexity. In Section 4 we study the iso-electronic series with the LMC complexity measure. Concrete similarities and differences between the various complexities and systems studied are pointed out.

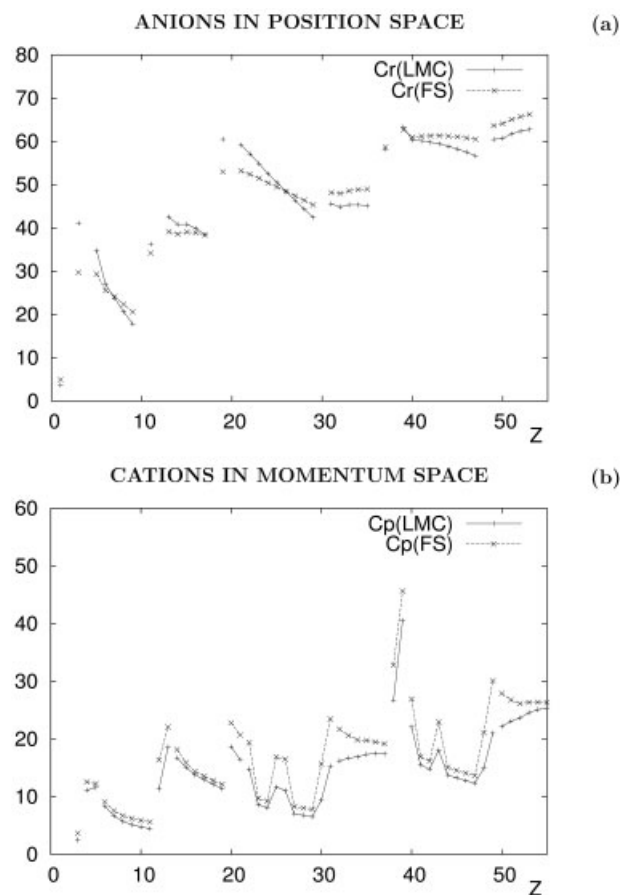


FIGURE 1. Complexities $C(\text{LMC})$ and $C(\text{FS})$ for (a) anions in position space, and (b) cations in momentum space, for singly charged ions with nuclear charge Z . Atomic units (a.u.) are used.

3. Complexity Analysis for Ionization Processes

In this section we first compare the Fisher-Shannon (FS) and López Ruiz–Mancini–Calbet (LMC) complexity measures followed in mono-ionization processes. In doing so we calculate the informational measures (i) (I, J) to construct $C(\text{FS}) = I \cdot J$, and (ii) (D, L) to construct $C(\text{LMC}) = D \cdot L$. We analyze a set of 150 atomic systems including anions, neutral species and cations. In Figure 1(a) we show both complexities, in position space, for anions, and in Figure 1(b), now for variety in momentum space, the same information measures for cations.

Both figures clearly display the strong structural similarity between $C(\text{LMC})$ and $C(\text{FS})$. Let us remark here that each complexity consists of two factors, one

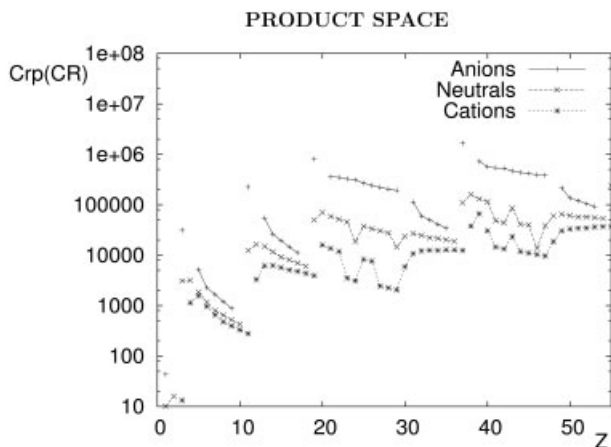


FIGURE 2. Complexity $C(\text{CR})$ in product space for neutral atoms and singly charged ions with nuclear charge Z . Atomic units (a.u.) are used.

of them always defined in terms of the Shannon entropy S , being the other factor that which characterizes more specifically the corresponding complexity, because we are using a global quantity (i.e., disequilibrium D) for $C(\text{LMC})$ but a local one (i.e., Fisher information) for $C(\text{FS})$. Nevertheless, there are no relevant structural differences between complexities based on the global or the local magnitude. Additionally, such a comment can be done independently of the conjugate space considered.

As it is apparent, not only the trends but also the numerical values of both magnitudes are very similar. This result contrasts with other previous ones, where diverse atomic information magnitudes must be arbitrarily factorized or scaled in order to carry out a useful comparison [23, 36].

Another relevant characteristics of all curves plotted in such Figures 1(a) and (b) are the strong correlation appearing between the process of shell-filling in atomic systems (and also the group the 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 few exceptions, $C(\text{LMC})$ and $C(\text{FS})$ 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 the values $Z = 24, 29, 46$, all characterized for losing an "s" electron). Also maxima are frequently associated to shell structure.

Concerning the behavior of the Cramer-Rao complexity $C(\text{CR}) = I \cdot V$ throughout the ionization

process, its dependence on the nuclear charge Z and correlation with atomic shell structure are clearly displayed in Figure 2 for the product space rp , in a compact and complete form. Total complexity increases while losing an electron with overall organization (with Z) but showing the characteristic trends of the shell structure. Maxima are clearly associated to "s" subshells, as happens with the relative minima in noble gases or some anomalous filling of "d" shells.

Figure 3(a) shows the Cramer-Rao Plane, i.e., the $I-V$ plane, in the position space for these systems. Some facts are worthy to remark in this figure. First, it is clear that the CR plane, apart from reproducing faithfully the atomic shell structure, reveals that systems of large Z are highly localized and organized whereas light systems have much more delocalization. Second, location at the plane after an ionization process for heavy atoms slightly changes when compared to those suffered by light atoms.

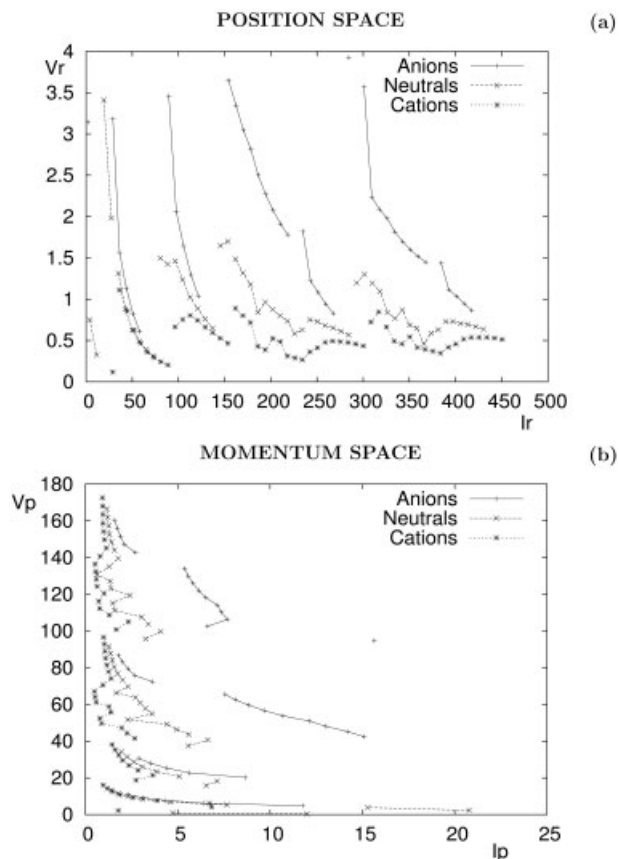


FIGURE 3. $I-V$ (Fisher-Variance) planes in (a) position and (b) momentum spaces, for neutral atoms and singly charged ions with nuclear charge Z . Atomic units (a.u.) are used.

Furthermore, complexity for a given Z decreases following the sequence anion-neutral atom-cation, i.e. as losing electrons. Third, ionization in “s” subshells are processes characterized by a considerable gain of complexity as compared to those in “p” or “d” subshells, which increases only moderately the product of I and V measures.

Figure 3(b) shows the I - V plane in the momentum space. It is important to note here that the behavior in this space is just the opposite than in r space. Systems of large Z are now less localized and have a greater value of variance, whereas light systems are more localized in p space. Besides in the process of loss of electrons the variance increases whereas I_p decreases, just the reciprocal that happens in r space.

It is important to remark that replacing Fisher information (which measures the gradient content of the density) by the global disequilibrium D (which measures the global density content), leading to the complexity $D \cdot V$, also shows very analogous trends to those of Cramer-Rao complexity.

4. Complexity Analysis of Isoelectronic Series

Let us focus now, not in the outer electronic layer like in the previous section, but in the core of the atom. We analyze nine isoelectronic series corresponding to $N = 2 - 10$ electron systems. Each series consists of 21 systems of equal electronic charge N , with nuclear charge running from $Z = N$ to $Z = N + 20$. In this way we study how complexity measures characterize, from the informational point of view, this set of 189 different systems. On one hand the effect of decreasing the nuclear charge Z from $N + 20$ to N is studied, and on the other the electronic organization of each isoelectronic series can also be investigated.

LMC-type measures are calculated for each isoelectronic series in position, momentum, and product spaces in order to compare them and have a more complete and accurate analysis of these systems. In this case we use the LMC measure, i.e. $C(\text{LMC}) = L \cdot D$. Results are displayed in a D vs. L plane: the disequilibrium-entropy plane.

Figures 4(a) and (b) show, respectively, the results in r and p spaces in a double logarithmic scale. Each isoelectronic series follows a D - L trajectory that can be easily analyzed. The isoelectronic series corresponding to He shows an almost constant $C(\text{LMC}) = D \cdot L$ line in both spaces, showing that

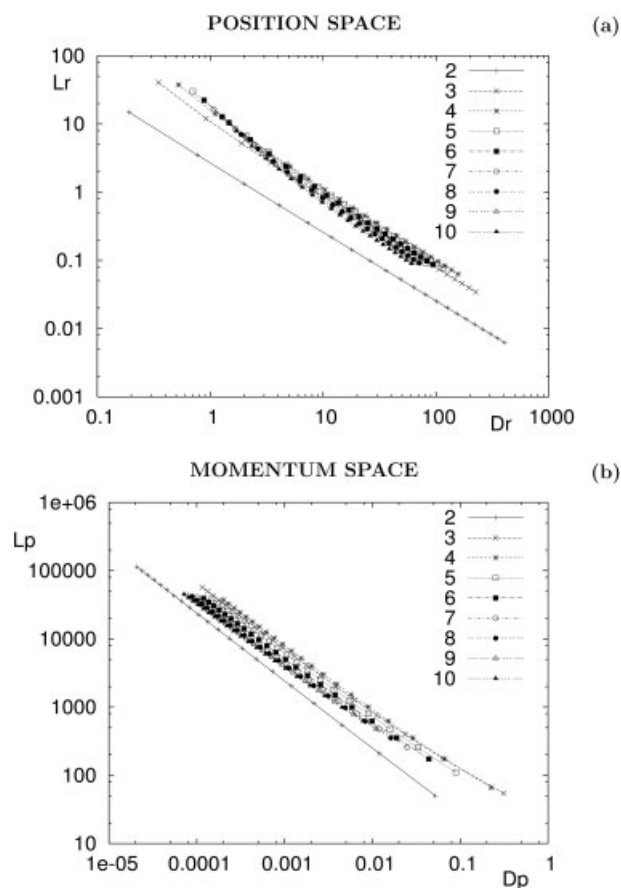


FIGURE 4. D - L (Disequilibrium-Exponential entropy) planes in (a) position and (b) momentum spaces, for isoelectronic series with 2–10 electrons. Atomic units (a.u.) are used.

the effect of increasing the nuclear charge produces, obviously, more localization (D) and consequently less uncertainty (L). However, this fact does not affect significantly the product measure $C(\text{LMC}) = D \cdot L$, where an increase (decrease) in uncertainty (L) is compensated by a proportional decrease (increase) of localization (D).

Systems with large nuclear charge Z in r space [Fig. 4(a)] are located in the right-lower corner of the figure, showing a highly localized structure (D large), independently of the isoelectronic series they belong to. The trajectories of the isoelectronic series in this zone show that the product measure there is almost constant. However, when nuclear charge decreases, systems deviate from the constant isoproduct lines and show greater complexity. Neutral systems (on the left-upper zone of the D - L plane), breaking definitely this false linearity, possess the biggest complexity in r space and are char-

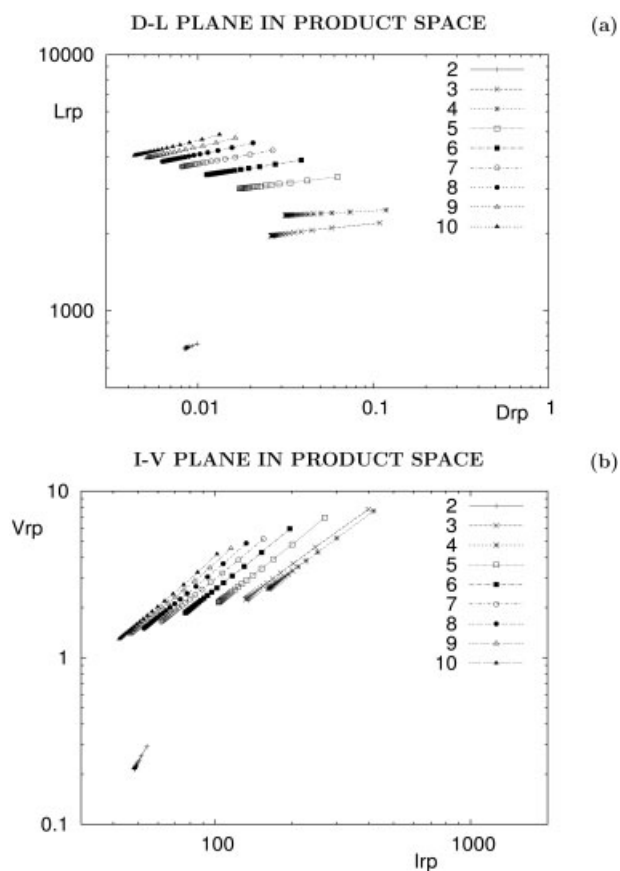


FIGURE 5. (a) D - L (Disequilibrium-Exponential entropy) and (b) I - V (Fisher-Variance) planes in product space, for isoelectronic series with 2–10 electrons. Atomic units (a.u.) are used.

acterized by a relatively lower localization and greater uncertainty when compared to members of their same series.

It is interesting to note the exact reciprocal behavior displayed by all series in the complementary p space [Fig. 4(b)]. Now systems of large nuclear charge are located in the left-upper zone of the figure, showing a low localization in momentum space and high entropy, whereas neutral systems are located in the low entropy and high localization region and show a deviation from the isoproduct lines that implies, as in the r case, the biggest structure/complexity.

The distance between systems within the same isoelectronic series falls with increasing Z , giving rise to a higher similarity between systems with large nuclear charge; on the contrary, systems with low Z separate progressively, showing different trends. Figure 5(a) presents the L vs. D trajectories

of the nine isoelectronic series in the product space. It is important to remark now the radical change in the slopes of all series compared to those of isolated r and p planes. Systems with heavy nuclei are on the lower part of the figure and neutral systems on the upper one. Once again neutral systems show more complexity than the cations of its series. The shell structure is now clearly perceptible, showing for instance that systems filling the $2s$ subshell display more complexity than those filling the $2p$ subshell. Also noble gases show the smallest complexity compared to other atoms.

Similar results to those discussed above are also obtained when using the Cramer-Rao plane (i.e., V vs. I plane), as shown in Figure 5(b). Those comments are also valid when studying additional information planes (e.g., I vs. L or L vs. V), which corresponding figures are not included in the present work for the sake of simplicity.

5. Conclusions

LMC-type complexity measures detecting not only randomness but also structure and organization are defined and subsequently computed using near Hartree–Fock wave functions for neutral atoms, anions, and cations with nuclear charge $Z = 1$ –54 in position, momentum and product spaces (150 systems). Besides the complexity content of nine isoelectronic series, (189 systems) is analyzed with these information theoretic products consisting of two factors, a localization (I or D) and a delocalization (V , S , L , or J) one.

The localization–delocalization planes are useful to represent the informational trajectories of the different processes or systems under investigation and the complementary use of r and p spaces provides a compact and more complete understanding of the information content of these planes.

It is shown that FS and LMC complexities (using very different first localization factors, a local and a global one, respectively) are qualitatively and numerically equivalent for all these systems, and that the other LMC-type complexities give similar qualitative results. In particular the Cramer-Rao complexity $I \cdot V$, defined in terms of the complementary factors of the LMC one $L \cdot D$, is a relevant candidate to investigate the pattern of a system or process.

Concretely we study the informational effect of increasing or decreasing the nuclear charge in isoelectronic series. It is shown that behaviors in r and p spaces are just the opposite within each isoelectronic

series. The joint behavior in rp space shows more clearly the increase in complexity as far as the nuclear charge decreases.

Concerning the mono-ionization processes the whole structure of the periodic table according to shell-filling is revealed. Again the trends in conjugate spaces are opposite one to the other. All LMC-type complexities are ordered for fixed Z according to the global charge, being larger for anions and lower for cations, with neutral systems in the middle. LMC-type complexities increase, in overall, with nuclear charge Z , but local maxima appear associated to systems filling ns subshells, corresponding noble gases to relative minima.

As main conclusion, one cannot use only a measure of uncertainty/randomness or a measure of concentration/localization to measure the informational content or the organization of a system. Measures like LMC-type complexities that take into account both faces seem more suitable to describe the complexity of an atomic or, in general, a multi-fermionic system.

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