

Fisher-Shannon analysis of ionization processes and isoelectronic seriesK. D. Sen,¹ J. Antolín,^{2,4} and J. C. Angulo^{3,4}¹*School of Chemistry, University of Hyderabad, Hyderabad-500046, India*²*Departamento de Física Aplicada, EUITIZ, Universidad de Zaragoza, 50009-Zaragoza, Spain*³*Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada, 18071-Granada, Spain*⁴*Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, 18071-Granada, Spain*

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The Fisher-Shannon plane which embodies the Fisher information measure in conjunction with the Shannon entropy is tested in its ability to quantify and compare the informational behavior of the process of atomic ionization. We report the variation of such an information measure and its constituents for a comprehensive set of neutral atoms, and their isoelectronic series including the mononegative ions, using the numerical data generated on 320 atomic systems in position, momentum, and product spaces at the Hartree-Fock level. It is found that the Fisher-Shannon plane clearly reveals shell-filling patterns across the periodic table. Compared to position space, a significantly higher resolution is exhibited in momentum space. Characteristic features in the Fisher-Shannon plane accompanying the ionization process are identified, and the physical reasons for the observed patterns are described.

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I. INTRODUCTION

Shannon entropy [1] (S) and the Fisher information measure [2] (I) of the probability distributions are becoming increasingly important tools of scientific analysis in a variety of disciplines of scientific enquiry. Jaynes' maximum entropy principle, which utilizes S , provides a method for constructing the whole of statistical thermodynamics [3] which has led to a large variety of applications centered around S . On the other hand, the Frieden extreme physical information principle [4] uses the Fisher information measure to derive important laws of chemistry and physics [5], such as the equations of the nonrelativistic quantum mechanics [6] or relevant results in density functional theory [7,8]. While the Shannon entropy has remained the major tool in information theory, there have been noteworthy applications of Fisher information [7–12]. Overall, these studies suggest that both S and I can be used as complementary tools to describe the information behavior, pattern, or complexity of physical systems and the electronic processes involving them.

Measuring the complexity of a general system is yet another interesting area of contemporary research which has roots in information theory. One of the proposals due to López-Ruiz, Mancini, and Calbet (LMC) [13] defines the statistical complexity measure simply as the product of disequilibrium and the Shannon entropy of the probability distribution. Here, the disequilibrium is defined as the expectation value of the probability density (quadratic distance from the equiprobability). The LMC measure has been criticized [15,16] and modified, leading to the definition of *shape* complexity [17,18], which satisfies several desirable properties of invariance under scaling, translation, and replication and has been further generalized [19,20] to include Rényi and Tsallis entropy measures. The utility of such generalized complexity measures has been demonstrated recently [21,22]. 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 [23], both of which are

expressed in terms of Shannon entropy values.

In view of the fact that for a normal distribution the Fisher measure estimates the inverse of variance and the disequilibrium defined as the density expectation value measures the square root of inverse variance, it is possible, in principle, to employ Shannon entropy in conjunction with Fisher information to describe the complexity of atomic systems and study their associated electronic properties such as ionization and polarizability. Relative to the LMC measure, using the Fisher-Shannon plane as a measure of complexity offers the advantage of (a) incorporating a global measure of uncertainty (Shannon) and a local or intrinsic measure of accuracy (Fisher) and (b) obtaining a higher sensitivity particularly where the density oscillations are involved. This has motivated us to study the Fisher-Shannon plane to describe the ionization process in the position and momentum spaces. We note here that the Shannon entropies in the position and momentum spaces alone were used earlier [24] to study the electron correlation effects in the He, Li, Be, and Ne isoelectronic series. The Fisher-Shannon plane has been applied successfully to various fields—e.g., to the analysis of signals [25] and the study of electron correlation [26] within the He-isoelectronic series. Other similar analyses have been done using the well-known Cramer-Rao plane where the involved magnitudes are the variance and the Fisher information of the distribution [27,28].

The aim of this work is to carry out a comprehensive analysis in the Fisher-Shannon plane for simple, but strongly organized N -electronic systems ($N=2-54$) of neutral atoms and their singly charged ions. In particular, we have studied (a) the behaviors in the Fisher-Shannon plane accompanying the process of gain or loss of one electron for an atom at constant Z and (b) the isoelectronic variation of this information measure of over a fairly extended range of Z values. Both partial variations with respect to the electron number N and the nuclear charge Z are found to show characteristic features in the Fisher-Shannon plane. This study tests the feasibility of using the Fisher-Shannon plane as a

information-theoretical tool to describe changes in the electronic density as a function of electron number N and nuclear charge Z , respectively. The outline of this paper is as follows. In Sec. II the defining tools of carrying out the Fisher-Shannon analysis are presented. Sections III and IV present and discuss the results of such analyses on the isoelectronic changes and ionization, respectively. Finally, in Sec. V we have summarized the main conclusions of the present work.

II. FISHER-SHANNON PLANE FOR ELECTRONIC DENSITIES

The study of the main physical properties of many fermion systems involves, as basic variables, the one-particle densities in both position and momentum spaces, $\rho(\mathbf{r})$ and $\Pi(\mathbf{p})$, respectively, as shown in the density functional theory [29]:

$$\rho(\mathbf{r}) = \int |\Psi(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N)|^2 d\mathbf{r}_2 \cdots d\mathbf{r}_N, \quad (1)$$

$$\Pi(\mathbf{p}) = \int |\Phi(\mathbf{p}, \mathbf{p}_2, \dots, \mathbf{p}_N)|^2 d\mathbf{p}_2 \cdots d\mathbf{p}_N, \quad (2)$$

where $\Psi(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N)$ denotes the normalized wave function of the N -electron system, $\Phi(\mathbf{p}, \mathbf{p}_2, \dots, \mathbf{p}_N)$ is its Fourier transform, and all densities are normalized to unity.

As we have pointed out before, information theory is being applied successfully to the study of the electronic structure of atoms and molecules. We use in this case *Shannon entropy* and *Fisher information* S_r and I_r in position space \mathbf{r} , defined, respectively, by

$$S_r = - \int \rho(\mathbf{r}) \ln \rho(\mathbf{r}) d\mathbf{r} = - \langle \ln \rho(\mathbf{r}) \rangle, \quad (3)$$

$$I_r = \int [|\nabla \rho(\mathbf{r})|^2 / \rho(\mathbf{r})] d\mathbf{r} = \langle |\nabla \ln \rho(\mathbf{r})|^2 \rangle \quad (4)$$

($\langle \cdot \rangle$ denotes the expectation value). Their momentum-space counterparts S_p and I_p are defined in an analogous manner using instead of the charge density $\rho(\mathbf{r})$, the momentum density $\Pi(\mathbf{p})$.

In this study it is sufficient to deal with the spherically averaged electron densities $\rho(r)$ or $\Pi(p)$, each normalized to unity; therefore, we can use one-dimensional integrals.

There are a number of candidates for a direct measure of uncertainty or spread of a one-dimensional probability distribution $\rho(r)$, the most well known being the *variance* of the distribution $V = \sigma^2$ (σ is the root-mean-square deviation):

$$V = \sigma^2 = \langle r^2 \rangle - \langle r \rangle^2. \quad (5)$$

A second candidate, which shares all the virtues of σ (same units as r , translation and reflection invariance, linear scaling, and vanishing when approaching a δ function) is the *inverse participation ratio* or *informational energy* [30],

$$\frac{1}{D} = \left[\int \rho^2(r) dr \right]^{-1} = \langle \rho(r) \rangle^{-1}. \quad (6)$$

D , which, as noted earlier, behaves like the inverse of σ , is also used in many different fields to represent the Onicescu information energy [31], *self-similarity* [32], *disequilibrium* [13], *purity* in quantum mechanics, or simply *average density*. $1-D$ is also called *dissimilarity* or *linear entropy* in contrast with the nonlinear Shannon entropy. It is also an experimentally measurable quantity [14].

However, the magnitude $1/D$ is in fact only a special case ($\alpha=1$) of what may be called *rényi lengths* [33], which are closely related to *rényi entropies* (its logarithm), and their reciprocals were also extensively investigated in Ref. [34]:

$$L_\alpha = \left[\int \rho^{\alpha+1}(r) dr \right]^{-1/\alpha}. \quad (7)$$

The so-called *exponential entropy*, denoted by $N_r = e^{S_r}$, guarantees positivity and is simply given by direct measure of spread L_α in the limit $\alpha \rightarrow 0$. Thus Shannon entropy (or power Shannon entropy) behaves like a measure of delocalization or lack of structure of the electronic density in the position space. Thus S_r is maximal when knowledge of $\rho(\mathbf{r})$ is minimal. This magnitude has been extensively used in the study of many-electron systems and a variety of important results have been obtained [35]. In particular, it has been related to the quality of the basis set [36] and correlation of the wave function [37] as well as many atomic and molecular properties [38]. Of course, in general, all the moments of the electronic density give information on the quantification of the spreading of the density around the origin. A variety of relations, bounds, and inequalities between them and other functionals of the density, or ever including the own density [39], are published [40].

It has been demonstrated that the (much less used) momentum density, particularly from an entropic perspective, provides complementary insight into chemical phenomena of atoms or molecules [41]. The Shannon entropy in momentum space is largest for systems where electrons are of undeterminable speed and is smaller for systems with a high proportion of relaxed atoms—i.e., low p . This momentum entropy S_p is closely related to S_r by the well-known uncertainty relation of Bialynicki-Birula and Mycielski [42], which shows that the sum of both entropies—i.e., $S_T = S_r + S_p$ —cannot decrease arbitrarily and is a balanced measure by taking into account the entropic boundary of the distribution in both spaces. The usual interpretation (in one-electron atomic systems) is that localization of the electron's position results in an increase in kinetic energy and a delocalization of the momentum density. A weak nuclear potential would imply a delocalized electron density and hence a localized electron momentum density [41] in n dimensions,

$$S_T = S_r + S_p \geq n(1 + \ln \pi), \quad (8)$$

generalizes the well-known Heisenberg bound $\langle r^2 \rangle \langle p^2 \rangle \geq n^2/4$. There are similar uncertainty inequalities that relate Rényi lengths as well as power entropies in position and momentum spaces [43].

It is worthy to mention that the generalized Shannon entropies such as Rényi [44], Tsallis [45], or Havrda-Charvat [46] entropies are less commonly used in the informational study of electron distributions. Similarly, Fisher information, which is a measure of the localization of distribution, has not been used until very recently to investigate directly electronic densities. However, it is a well-known statistical estimator and its role in information theory, density functional theory, and inverse problems was emphasized recently [7–12,47,48].

Besides, Fisher information fulfills important uncertainty relations such as the Cramer-Rao bound $IV \geq 1$ or the Stam uncertainty $I_r < 4V_p$ and $I_p < 4V_r$ [43]. Taking into account the previous bounds and simply redefining the entropy power as

$$J = \frac{1}{2\pi e} e^{(2/n)S}, \quad (9)$$

it has been shown [43] that

$$P \equiv IJ \geq n. \quad (10)$$

Some of the above information magnitudes have been recently used to analyze atomic systems and their properties. In [49] LMC and SDL complexities are compared for the neutral atoms ($2 \leq Z \leq 54$). The net Fisher information measure is found to correlate well with the inverse of the ionization potential and dipole polarizability [50]. Some studies on atomic similarity, using magnitudes closely related to D or to relative Shannon entropies, have been also reported [51,52]. Very recently a comparative analysis of I and D shows that they both vary similarly with Z within the neutral atoms, exhibiting the same maxima and minima, but Fisher information presents a significantly enhanced sensitivity in the position and momentum spaces in all systems considered [53].

In this work, the lower bound (10) to the product of these two important and complementary magnitudes (similar to the Cramer-Rao one) and the inverse behavior of I and J as measures of localization and uncertainty, respectively, as well as their inverse local and global meaning, suggest the use of a product measure $P=IJ$, in line with the $C_{LMC}=DS$ measure of complexity [13,17–19], which can be called the Fisher-Shannon measure. The trajectories of different electronic processes or systems can be easily represented in a J versus I plane where lines of equal Fisher-Shannon measure can recognize the different content of complexity, structure, and pattern of each process or system. To the best of our knowledge this (or closely related) Fisher-Shannon measure has been only applied in two previous studies [25,26]. Some more interesting properties of this product measure such as scaling and uncertaintylike relationships have been also examined [43].

As described in the Introduction, we apply the Fisher-Shannon measure to isoelectronic series of ions (Sec. III) and to monoionization processes (Sec. IV), in position ($P_r = I_r J_r$), momentum ($P_p = I_p J_p$), and product ($P_{rp} = I_{rp} J_{rp}$) spaces, where

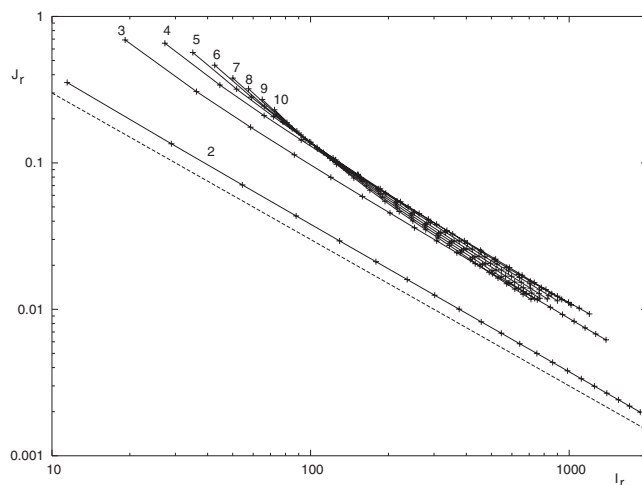


FIG. 1. Fisher-Shannon plane for isoelectronic series in r space. Double-logarithmic scale. Numbers in the graph indicate N —i.e., electrons of the series. Systems of large Z are on the lower-right zone of the figure. Neutral systems are in the upper-left zone. The dashed line shows the rigorous lower bound $IJ=3$ for $P=JI$. Atomic units (a.u.) are used.

$$P_{rp} = I_{rp} J_{rp} = I_r I_p J_r J_p = I_r I_p \frac{1}{2\pi e} e^{(2/n)(S_r+S_p)}. \quad (11)$$

In the computations the atomic wave functions of Koga *et al.* [54] have been employed to calculate the atomic densities and their corresponding informational measures for all the atomic systems.

III. FISHER-SHANNON ANALYSIS OF ISOELECTRONIC SERIES

Isoelectronic series studies provide a well-known benchmark for the study of atoms and molecules. In this section results concerning the application of the entropic functionals, defined previously, are presented. We have analyzed nine isoelectronic series corresponding to $N=2-10$ electron systems. Each series consists of 21 systems of equal electronic charge N and nuclear charge running from $Z=N$ to $Z=N+20$. In this form we study how Fisher-Shannon measure characterizes, from the informational point of view, this set of 189 different systems. On the one hand, the effect of decreasing nuclear charge (from $Z+N$ to N) can be studied and on the other the electronic organization of each isoelectronic series can be investigated.

Fisher and Shannon 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. We shall now present the results of our calculations as displayed in a J vs I plane—i.e., the Fisher-Shannon plane.

Figures 1 and 2 show, respectively, the results in r and p spaces in a double-logarithmic scale. Line $P=JI=3$, in both spaces, divides the Fisher-Shannon plane into two regions. The left area is the forbidden region by inequality (10), and parallel lines to it show isocomplexity processes showing

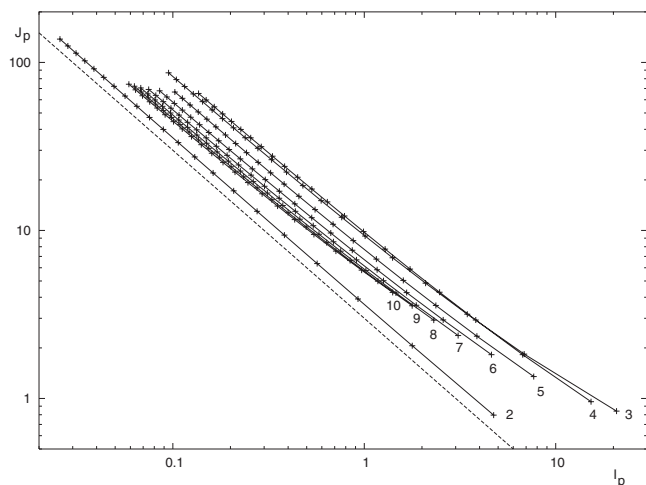


FIG. 2. Fisher-Shannon plane for isoelectronic series in p space. Double-logarithmic scale. Numbers in the graph indicate N —i.e., electrons of the series. Systems of large Z are on the upper-left zone of the figure. Neutral systems are in the lower-right zone. The dashed line shows the rigorous lower bound $IJ=3$ for $P=JI$. Atomic units (a.u.) are used.

that an increase (decrease) in uncertainty (J) in them is compensated for by a proportional decrease (increase) of accuracy (I). Each isoelectronic series follows a trajectory in the Fisher-Shannon plane that can be easily analyzed. The isoelectronic series corresponding to He shows an almost constant $P=4$ line in both spaces, showing that the effect of increasing the nuclear charge produces, obviously, more localization (I) and consequently less uncertainty (J). However this fact does not affect very much to the product measure, $P=JI$.

Systems with large nuclear charge in r space (Fig. 1) are located in the right-lower zone of the figure, showing a high localized structure (I large), independently of the isoelectronic series they belong. The trajectories of the isoelectronic series show that the product measure in this zone is almost constant. However, when nuclear charge is decreased, systems deviate from the constant isoproduct lines and show greater complexity. Neutral systems (on the left-upper zone of the J - I plane), breaking definitely this false linearity, show the largest complexity in r space and are characterized 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 suffered by all series in the complementary p space (Fig. 2). Now systems of large nuclear charge are located in the left-upper zone of the figure, showing a low- p localization in this space and high entropy; on the contrary, neutral systems are located in the low-entropy and high-localization region and show a deviation from the isoproduct lines, which implies as in the r case, the largest structure and complexity.

The distance between systems in the same isoelectronic series falls with Z , showing more similarity between systems with large nuclear charge; on the contrary, systems with low Z separate more and more, showing different trends.

Figure 3 presents the trajectories of the nine isoelectronic series in the product space. It is important to remark now the

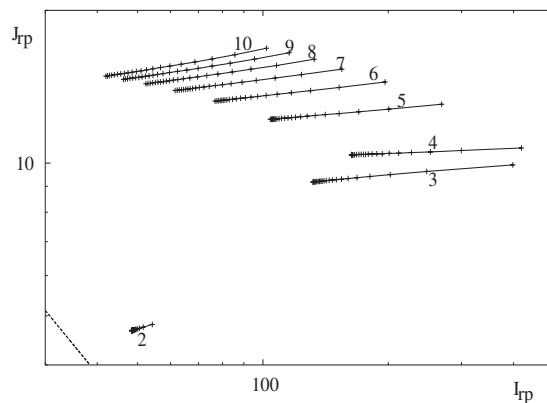


FIG. 3. Fisher-Shannon plane for isoelectronic series in product rp space. Double-logarithmic scale. Numbers in the graph indicate N —i.e., electrons of the series. Systems of large Z are on left zone of the figure. Neutral systems are in the right zone. The dashed line shows the rigorous lower bound $IJ=18\pi e$ for $P=JI$. Atomic units (a.u.) are used.

radical change in the slopes of all series in comparison with those of r and p planes. Systems with heavy nuclei are on the left and neutral systems on the right. Localization in this product (rp) plane is very different, whereas the joint entropy does not change so drastically. Once again neutral systems show more complexity than the cations of their series. The shell structure is now present, showing that systems filling the $2s$ subshell present more complexity than those filling the $2p$ subshell. Also noble gases show the smallest complexity compared with other atoms.

In Figs. 2 and 3, a different behavior is displayed by the $N=2$ series compared to the other series. This is due to the fact that $N=2$ series is unique in that it is devoid of a shell of core electrons. Equivalently, all electrons have principal quantum number $n=1$ in this series whereas for others a valence shell is introduced with $n=2$.

In conclusion, it is clear from these Figs. 1–3 that in addition to the independent studies in the position or momen-

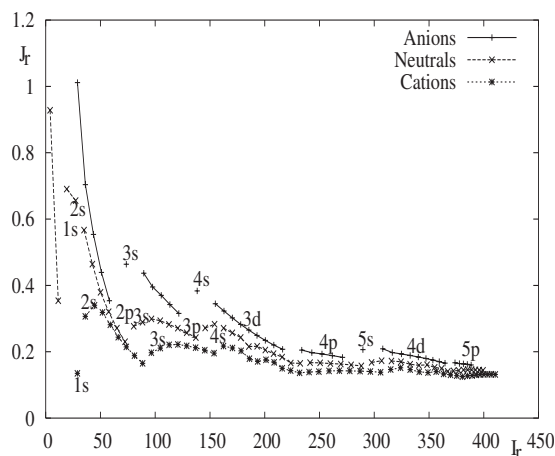


FIG. 4. Fisher-Shannon plane for ionization processes in r space. Linear scale. Numbers in the graph indicate the corresponding subshell. The dashed line shows the rigorous lower bound $IJ=3$ for $P=JI$. Atomic units (a.u.) are used.

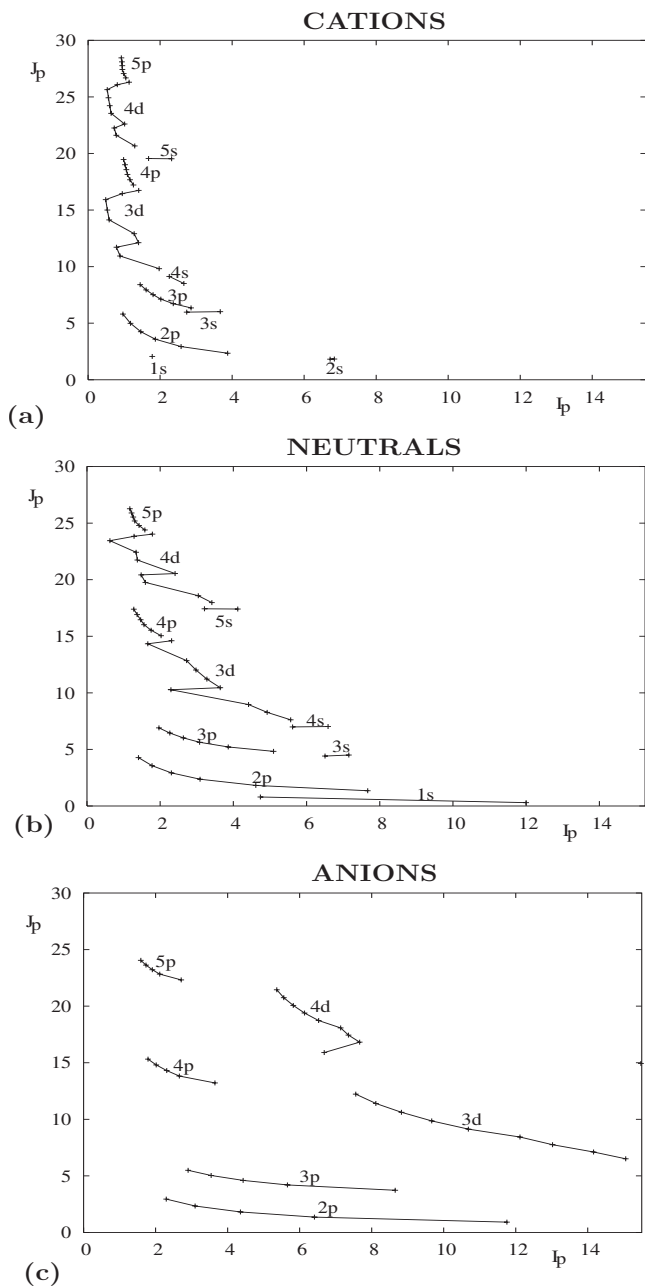


FIG. 5. Fisher-Shannon plane for ionization processes in p space. Triple figure. Linear scale. Numbers in the graph indicate the corresponding subshell. The dashed line shows the rigorous lower bound $IJ=3$ for $P=JI$. Atomic units (a.u.) are used.

tum space, the product-space behavior is important in itself. Further, a suitable combination of a measure of uncertainty (randomness) or a measure of concentration (localization), like, e.g., P , seems desirable to study the isoelectronic changes in the electronic density.

IV. FISHER-SHANNON PLANE FOR IONIZATION PROCESSES

In this section we study the Fisher-Shannon trajectories followed in monoionization processes. Then we focus now,

not in the core of the atom like in the previous section, but in the outer electronic layer. In doing so we calculate the informational measures: I , J , and P to analyze a set of 149 atomic systems including anions, neutral species, and cations.

In Fig. 4, and now in a linear scale, the Fisher-Shannon (FS) plane in position space is plotted for these systems. Some facts are worthy to remark on in this figure. First, it is clear that the FS plane reproduces faithfully the atomic shell structure, systems of large Z being highly localized and organized, whereas light systems have much more entropy. Second, changes in the ionization processes of heavy atoms are smaller than those suffered by light atoms. Furthermore, the complexity, for a given Z , is largest for the anion followed by neutral atoms and cations, respectively. Third, ionization in s subshells is a process 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 J measures.

Figures 5(a)–5(c) show the Fisher-Shannon plane in momentum space, separately for anions, neutrals, and cations, for more clarity. Again the reciprocal behavior in this space is the opposite that in r space. Systems of large Z are now less localized and have more entropy. Light systems are more localized in p space. Besides in the process of loss of electrons entropy increases whereas I_p decreases, which is just the reciprocal of r -space behavior.

It is important to remark that the same calculations for ionic systems are done using Shannon S , Rényi, or Tsallis entropies, showing similar results. In the same way, the use of disequilibrium D (6), instead of Fisher information, also shows analogous complexity [17] trends.

Finally, in Fig. 6, for variety, complexities of all these systems in the product space are shown. Total information content increases while losing an electron with overall organization (with Z) but showing the characteristic trends of the shell structure. Maxima in s subshells are notorious and also the relative minima in noble gases (or some anomalous filling in d shells).

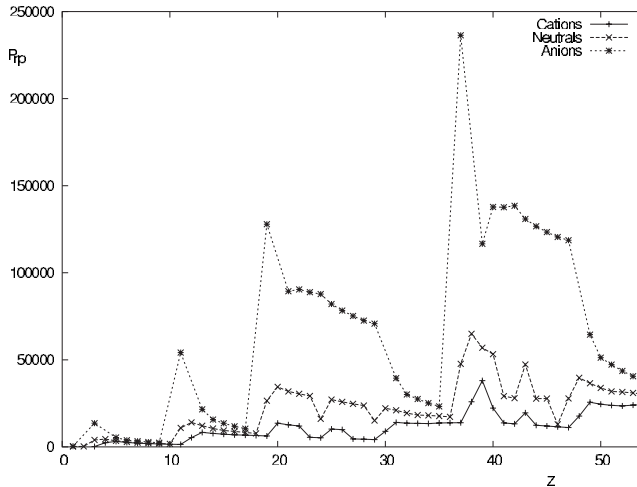


FIG. 6. Fisher-Shannon complexity ($P_{rp}=I_{rp}J_{rp}$) vs Z for ionization processes in rp space. Linear scale. Atomic units (a.u.) are used.

V. CONCLUSIONS

Fisher information and Shannon entropy are used together to construct a product informational measure ($P=JI$), taking into account global (J) and local (I) characteristics of the electronic densities. Besides, one factor (J) measures randomness or uncertainty whereas the other measures localization or intrinsic accuracy (I) in the corresponding electronic system. This product informational measure can be a new candidate for measuring the complexity or organization of systems and processes in a similar form than SDL or LMC complexities do. The Fisher-Shannon plane is useful to represent the informational trajectories of the different processes or systems under investigation.

Using the Fisher-Shannon measure, 320 atomic systems in position, momentum, and product spaces are analyzed. In concrete 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 for each isoelectronic series. The joint behavior in rp space

shows more clearly the increase in complexity when the nuclear charge is decreased.

Concerning the monoionization processes the whole structure of the periodic table is reproduced. Again the trends in r and p space are opposite. Fisher-Shannon complexity, for a given Z obeys the order that anion > neutral > cation. Fisher-Shannon complexity increases, overall, with Z but systems filling ns subshells present maxima and noble gases relative minima.

We finally conclude that in addition to r or p space, the information analysis in product space provides a more complete understanding of changes in N and Z for electronic systems.

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