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Comparison of SDL and LMC measures of complexity: Atoms as a testbed

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Abstract

The *simple* measure of complexity $\Gamma_{\alpha,\beta}$ of Shiner, Davison and Landsberg (SDL) and the *statistical* one C, according to López-Ruiz, Mancini and Calbet (LMC), are compared in atoms as functions of the atomic number Z. Shell effects i.e. local minima at the closed shells atoms are observed, as well as certain qualitative trends of $\Gamma_{\alpha,\beta}(Z)$ and $C(Z)$. If we impose the condition that Γ and C behave similarly as functions of Z, then we can conclude that complexity increases with Z and for atoms the strength of disorder is $\alpha \simeq 0$ and order is $\beta \simeq 4$.

Keywords: Complexity; Information entropy

1. Introduction

There are various measures of complexity in the literature. A quantitative measure of complexity is useful to estimate the ability of a variety of physical or biological systems for organization. According to [1] a complex world is interesting because it is highly structured. Some of the proposed measures of complexity are difficult to compute, although they are intuitively attractive, e.g. the algorithmic complexity [2,3] defined as the length of the shortest possible program necessary to reproduce a given object. The fact that a given program is indeed the shortest one, is hard to prove. In contrast, there is a class of definitions of complexity, which can be calculated easily i.e. the *simple* measure of complexity $\Gamma_{\alpha,\beta}$ according to Shiner, Davison, Landsberg (SDL) [4], and the *statistical* measure of complexity C, defined by López-Ruiz, Mancini, Calbet (LMC) [5–7].

Whereas the perfect measure of complexity is as yet unknown, the present work reports analysis of electron densities at atoms. We specially refer to the shell structure (periodicity), using two of the simplest of complexity measures, SDL and LMC calculated as functions of the atomic number Z. This is a continuation of our previous work [8]. Those measures have been criticized in the literature [9–11] and a discussion is presented in Section 4.

Our calculations are facilitated by our previous experience and results for the information entropy in various quantum systems (nuclei, atoms, atomic clusters and correlated atoms in a trap-bosons) [8,12–21]. A remarkable result is the universal property for the information entropy $S = a + b \ln N$ where N is the number of particles of the quantum system and a, b are constants dependent on the system under consideration [13]. In fact, if one has a physical model yielding probabilities which describe a system, then one can use them to find S and consequently calculate the complexity of the system (in our case the atom) as function of Z. This was done in [8], where we calculated the Shannon information entropies in position-space (S_r) and momentum-space (S_k) and their sum $S = S_r + S_k$ as functions of the atomic number Z ($2 \leqslant Z \leqslant 54$) in atoms. Roothaan–Hartree–Fock electron wave functions (RHF), for $1 < Z \leqslant 54$, were employed [22]. For $Z = 1$ there is no electron–electron effect. Higher values of Z ($Z > 54$), due to the relativistic effects, are not considered. Analytic wavefunctions are available in [22] only for Z up to 54. Their importance lays in the fact that we can derive accurate wavefunctions in momentum space; in order to assure that the integration is accurate. In [8] we calculated the SDL measure with RHF densities for $1 \leqslant Z \leqslant 54$. In the present work we calculate LMC mea-

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sure in the same region of Z, for the sake of comparison. One could consider the case of Hartree–Fock wavefunctions for the extended region $1 < Z \leqslant 102$ [23]. It turns out that both cases are satisfactory (work in progress).

In [8] and the present work, we examine if complexity of an atom is an increasing or decreasing function of Z. This is related with the question whether physical or biological systems are able to organize themselves, without the intervention of an external factor, which is a hot subject in the community of scientists interested in complexity.

However, special attention should be paid with respect to the meaning of complexity or structure, which may depend on the system under consideration. In the case of atoms, the overall electrons through pair-wise electron–electron interaction under the external nuclear potential, lead to the characteristic electron probability distribution. The selected information measure which shows up in this manner is employed to estimate complexity. Periodicity is clearly revealed here.

In Section 2 we review briefly measures of information content and complexity. Section 3 contains our numerical results for the LMC measure and discussion. In Section 4 we comment on the validity of SDL and LMC measures.

2. Measures of information content and complexity of a system

The class of measures of complexity considered in the present work have two main features i.e. they are easily computable and are based on previous knowledge of information entropy S.

The Shannon information entropy in position space S_r is

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

where $\rho(\mathbf{r})$ is the electron density distribution normalized to one. The corresponding information entropy S_k in momentum space is defined as

$$S_k = -\int n(\mathbf{k}) \ln n(\mathbf{k})\, d\mathbf{k}, \tag{2}$$

where $n(\mathbf{k})$ is the momentum density distribution normalized to one.

The total information entropy is

$$S = S_r + S_k, \tag{3}$$

and it is invariant to uniform scaling of coordinates, i.e. does not depend on the units used to measure $\mathbf{r}$ and $\mathbf{k}$, while the individual S_r and S_k do depend [13].

S represents the information content of the quantum system (in bits if the base of the logarithm is 2 or nats if the logarithm is natural). For a discrete probability distribution $\{p_i\}_{i=1,2,\ldots,k}$, one defines instead of S, the corresponding quantities H and $H_{\max}$

$$H = -\sum_{i=1}^{k} p_i \ln p_i \quad \left(\sum_i p_i = 1\right) \tag{4}$$

and

$$H_{\max} = \log k. \tag{5}$$

The uniform (equiprobable) probability distribution $p_1 = p_2 = \cdots = p_k = \frac{1}{k}$, gives the maximum entropy of the system. It is noted that the value of $H_{\max}$ can be lowered if there is a constraint on the probabilities $\{p_i\}$.

Another measure of the information content of a quantum system is the concept of information energy E defined by Onicescu [24], who tried to define a finer measure of dispersion distribution than that of Shannon information entropy. Onicescu's measure is discussed in [8].

For a discrete probability distribution $(p_1, p_2, \ldots, p_k)$, E is defined as

$$E = \sum_{i=1}^{k} p_i^2, \tag{6}$$

while for a continuous one $\rho(x)$ is defined by

$$E = \int \rho^2(x)\, dx. \tag{7}$$

One can define a measure for information content analogous to Shannon's S by the relation

$$O = \frac{1}{E}. \tag{8}$$

For three-dimensional spherically symmetric density distributions $\rho(\mathbf{r})$ and $n(\mathbf{k})$, in position- and momentum-spaces respectively, one has

$$E_r = \int_0^\infty \rho^2(r) 4\pi r^2\, dr, \tag{9}$$

$$E_k = \int_0^\infty n^2(k) 4\pi k^2\, dk. \tag{10}$$

The product $E_r \cdot E_k$ is dimensionless and can be considered as a measure of dispersion or concentration of a quantum system. S and E are reciprocal. Thus we can redefine O as

$$O = \frac{1}{E_r E_k}, \tag{11}$$

in order to be able to compare S and E.

Landsberg [25] defined the order parameter Ω (or disorder Δ) as

$$\Omega = 1 - \Delta = 1 - \frac{S}{S_{\max}}, \tag{12}$$

where S is the information entropy (actual) of the system and $S_{\max}$ the maximum entropy accessible to the system. It is noted that $\Omega = 1$ corresponds to perfect order and predictability while $\Omega = 0$ means complete disorder and randomness.

In [4] a measure of complexity $\Gamma_{\alpha,\beta}$ was defined of the form

$$\Gamma_{\alpha,\beta} = \Delta^\alpha \Omega^\beta = \Delta^\alpha (1-\Delta)^\beta = \Omega^\beta (1-\Omega)^\alpha, \tag{13}$$

which is called the "simple complexity of *disorder* strength α and *order* strength β". One has a measure of category I if $\beta = 0$