

# Statistical measures applied to metal clusters: evidence of magic numbers

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## Abstract

In this work, a shell model for metal clusters up to 220 valence electrons is used to obtain the fractional occupation probabilities of the electronic orbitals. Then, the calculation of a statistical measure of complexity and the Fisher-Shannon information is carried out. An increase of both magnitudes with the number of valence electrons is observed. The shell structure is reflected by the behavior of the statistical complexity. The magic numbers are indicated by the Fisher-Shannon information. So, as in the case of atomic nuclei, the study of statistical indicators also unveil the existence of magic numbers in metal clusters.

*Key words:* Statistical Indicators; Metal Clusters; Shell Structure; Magic Numbers  
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Nowadays the calculation of information-theoretic measures on quantum systems has received a special attention [1,2,3]. The application of these indicators to atoms or nuclei reveals some properties of the hierarchical organization of these many-body systems [4,5]. In particular, entropic products such as Fisher-Shannon information and statistical complexity present two main characteristics when applied to the former systems. On one hand, they display an increasing trend with the number of particles, electrons or nucleons. On the other hand, they take extremal values on the closure of shells. Moreover, in the case of nuclei, the trace of magic numbers is displayed by these statistical magnitudes [6].

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Metal clusters are useful quantum systems to understand how the physical properties evolve in the transition from atom to molecule to small particle to bulk solid [7,8]. They also present a shell structure where it can be applied the statistical indicators before mentioned. As in the case of atoms and nuclei, the fractional occupation probabilities of valence electrons in the different orbitals can capture the shell structure. This set of probabilities can be used to evaluate the statistical quantifiers for metallic clusters as a function of the number of valence electrons. Similar calculations have been reported for the electronic atomic structure [4,5] and for nuclei [6]. In this work, by following this method, we undertake the calculation of statistical complexity and Fisher-Shannon information for metal clusters.

The jellium model provides an accurate description of some simple metal clusters. In this model, a valence electron is assumed to interact with the average potential generated by the other electrons and the ions [7,8]. The confinement potential in the Schrödinger equation leading to shell structure is taken as a potential intermediate between the three-dimensional harmonic oscillator and the three-dimensional square well. This yields a filling of shells with a number  $N$  of valence electrons given by the series: 2, 8, 18, 20, 34, 40, 58, 68, 70, 92, 106, 112, 138, 156, 166, 168, 198, 220 and so on. Each shell is given by  $(nl)^w$ , where  $l$  denotes the orbital angular momentum ( $l = 0, 1, 2, \dots$ ),  $n$  counts the number of levels with that  $l$  value, and  $w$  is the number of valence electrons in the shell,  $0 \leq w \leq 2(2l + 1)$ .

As an example, we explicitly give the shell configuration of a metal cluster formed by  $N = 58$  valence electrons. It is obtained:

$$(N = 58) : (1s)^2(1p)^6(1d)^{10}(2s)^2(1f)^{14}(2p)^6(1g)^{18}. \quad (1)$$

The fractional occupation probability distribution of electron orbitals  $\{p_k\}$ ,  $k = 1, 2, \dots, \Pi$ , being  $\Pi$  the number of shells, can be defined in the same way as it has been done for calculations in atoms and nuclei [4,5,6]. This normalized probability distribution  $\{p_k\}$  ( $\sum p_k = 1$ ) is easily found by dividing the superscripts  $w$  by the total number  $N$  of electrons. Then, from this probability distribution, the different statistical magnitudes (Shannon entropy, disequilibrium, Fisher information, statistical complexity and Fisher-Shannon entropy) can be obtained.

Here, we undertake the calculation of entropic products, a statistical measure of complexity  $C$  and the Fisher-Shannon entropy  $P$ , that result from the product of two statistical quantities, one of them representing the information content of the system, and the other one giving an idea of how far the system is from the equilibrium. The classical indicator of information is the Shannon

entropy, that in the discrete version is expressed as

$$S = - \sum_{k=1}^{\Pi} p_k \log p_k . \quad (2)$$

Any monotonous function of  $S$  can also be used for this purpose, such as the exponential Shannon entropy [9],  $H = e^S$  or  $J = \frac{1}{2\pi e} e^{2S/3}$ . The indicator of how much concentrated is the probability distribution of the system can be related with some kind of distance to the equilibrium distribution, that in our case is the equiprobability. The disequilibrium  $D$  given by

$$D = \sum_{k=1}^{\Pi} (p_k - 1/\Pi)^2 , \quad (3)$$

and the Fisher information  $I$  by

$$I = \sum_{k=1}^{\Pi} \frac{(p_{k+1} - p_k)^2}{p_k} , \quad (4)$$

where  $p_{\Pi+1} = 0$ , are two useful parameters in this direction. Then, the statistical measure of complexity,  $C$ , the so-called LMC complexity [10,11], is defined as

$$C = H \cdot D , \quad (5)$$

and the Fisher-Shannon information [12,13,14],  $P$ , is given by

$$P = J \cdot I . \quad (6)$$

The statistical complexity,  $C$ , of metal clusters as a function of the number of valence electrons,  $N$ , is given in Fig. 1. We can observe in this figure that this magnitude fluctuates around an slightly increasing average value  $N$ . This trend is also found for the electronic structure of atoms [5] and for the shell structure of nuclei [6], reinforcing the idea that in general complexity increases with the number of units forming a system. However, the shell model supposes that the system encounters certain ordered rearrangements for some specific number of units (electrons or nucleons) that coincide with closed shells. In the present case, this fact is reflected by the notable increase of  $C$  in the metal clusters with one valence electron more than those with closed shells, which are indicated in Fig. 1, just as happens for atoms when one electron is added to noble gases or when one nucleon is added to a closed shell in nuclei. Observe that some major shells do not show local minima at their closing. This effect is due to the number of valence electrons belonging to each shell: a shell with a few valence electrons displays a local minimum of  $C$  when is closed, but this is not the case when the number of valence electrons in a shell increases.

The Fisher-Shannon entropy,  $P$ , of metal clusters as a function of  $N$  is given in Fig. 2. It presents an increasing trend with  $N$ . The spiky behavior of  $C$

provoked by the shell structure is still present for  $P$  but becomes smoother in this case.  $P$  displays notable peaks only at a few  $N$  related with the filling of some major shells, concretely at the numbers 2, 8, 18, 34, 58, 92, 138, 198. It must be remarked that, similarly as happens with  $C$ , the maximum values of  $P$  are taken on the nuclei with one unit more than the former series, although now the difference is slightly appreciable. Only peaks at 20 and 40 disagree with the sequence of magic numbers {2, 8, 18, 20, 34, 40, 58, 92, 138, 198} obtained from experimental data, for instance, for  $Na$  clusters [15] and for  $Cs$  clusters [16,17]. Let us observe that the magic numbers are basically marked by the Fisher information such as it can be seen in Fig. 3.

In summary, the behavior of the statistical complexity  $C$  and the Fisher-Shannon information  $P$  with the number of valence electrons in metal clusters has been reported. The increasing trend of these magnitudes with the number of valence electrons,  $N$ , has been found. The method that uses the fractional occupation probabilities has been applied to calculate these statistical indicators. As in the case of atoms and nuclei, the shell structure is well displayed by the spiky behavior of  $C$ . On the other hand,  $P$  shows a smoother behavior but with relevant peaks just on the major shells that coincide with the series of magic numbers in metal clusters. Therefore, the qualitative study of metal clusters by means of statistical indicators unveil certain physical properties of them. In fact, we can conclude that this type of statistical measures is able to enlighten some conformational aspects of quantum many-body systems.

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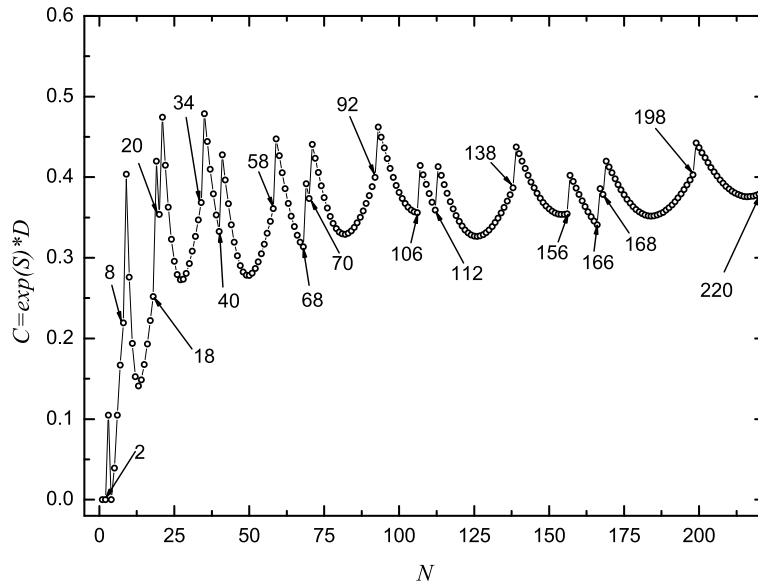


Fig. 1. Statistical complexity,  $C$ , vs. number of valence electrons,  $N$ . The arrows indicate the positions of closed shells.

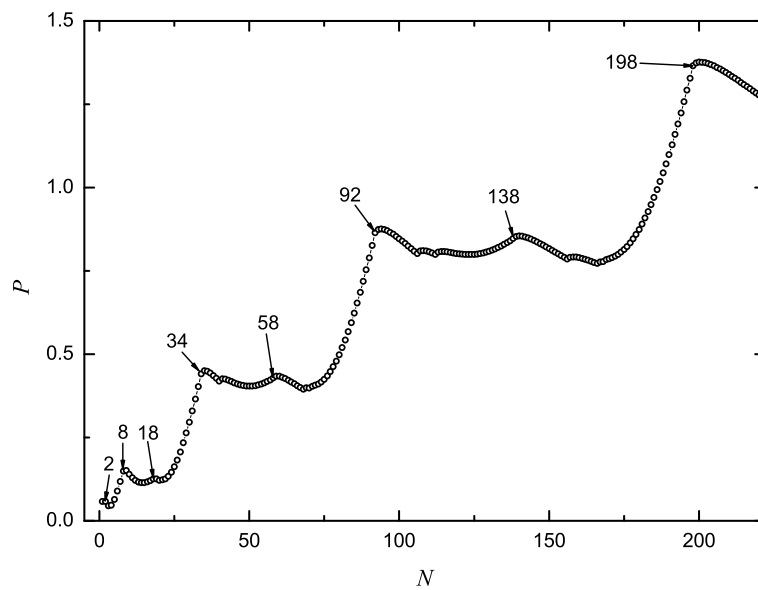


Fig. 2. Fisher-Shannon entropy,  $P$ , vs. the number of valence electrons,  $N$ . The arrows indicate prominent closed shells that are magic numbers. For details, see the text.

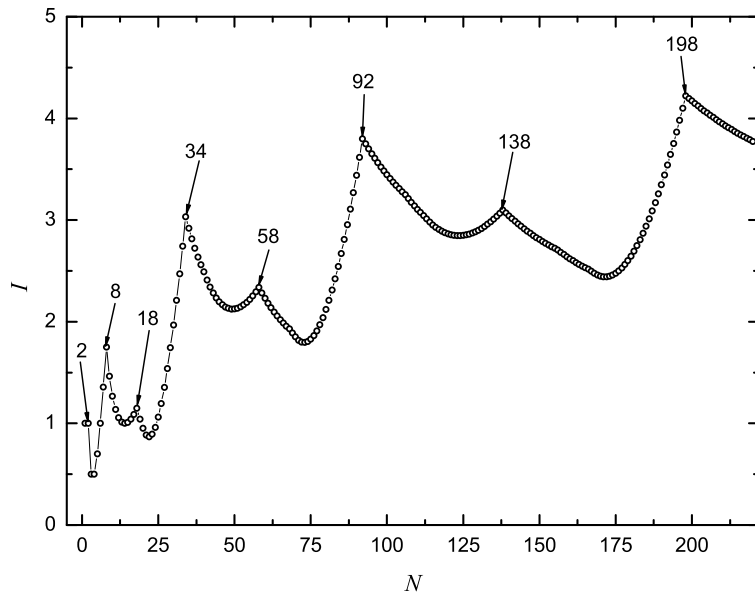


Fig. 3. Fisher information,  $I$ , vs. the number of valence electrons,  $N$ . The arrows indicate prominent closed shells that are magic numbers.