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Research Article

Complexity Measures for Maxwell–Boltzmann Distribution

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This work presents a discussion about the application of the Kolmogorov; López-Ruiz, Mancini, and Calbet (LMC); and Shiner, Davison, and Landsberg (SDL) complexity measures to a common situation in physics described by the Maxwell–Boltzmann distribution. The first idea about complexity measure started in computer science and was proposed by Kolmogorov, calculated similarly to the informational entropy. Kolmogorov measure when applied to natural phenomena, presents higher values associated with disorder and lower to order. However, it is considered that high complexity must be associated to intermediate states between order and disorder. Consequently, LMC and SDL measures were defined and used in attempts to model natural phenomena but with the inconvenience of being defined for discrete probability distributions defined over finite intervals. Here, adapting the definitions to a continuous variable, the three measures are applied to the known Maxwell–Boltzmann distribution describing thermal neutron velocity in a power reactor, allowing extension of complexity measures to a continuous physical situation and giving possible discussions about the phenomenon.

1. Introduction

The ordinary sense of complexity means complication, i.e., difficulty to understand or to deal with a system or device. Thinking in this way, Kolmogorov presented the concept of computational complexity [1], related to memory capacities and processing algorithms. However, new ideas started to be associated with complexity, statistical distributions, and information, mainly in life sciences [2–4].

Considering that natural systems are generally open and present emergence of global behaviors not decomposable into simpler parts [5–7], it seems that complexity is maximized for systems in the halfway of the equilibrium (disorder) and disequilibrium (order) [8]. Based on this, a seminal paper [9] proposed the LMC (López-Ruiz, Mancini, and Calbet) complexity measure for statistic distributions [10], with informational entropy [11] evaluating equilibrium, and deviation from the uniform distribution measuring disequilibrium.

Developing applications of thermodynamic entropy to measure disorder and complexity, Landsberg and Shiner studied how to contextualize this idea for the case of a nonequilibrium Fermi gas [12]. Then, Shiner et al. proposed a simplified version related to the LMC measure, replacing the disequilibrium term by the complement of the equilibrium term. This measure is called SDL (Shiner et al.) [13] and presents conclusions similar to that obtained by using LMC, for the majority of usual statistical distributions [14].

It was pointed out by Crutchfield et al. that an equilibrium system can be structurally complex [15], and this fact is not considered in LMC and SDL measures. The suggestion to solve this problem was presented in [16], considering that it is possible to introduce weights for order and disorder, according to the specific problem to be analyzed.

However, the main criticism comes from the experimentalists that question the usefulness of the approach in providing new insights for studying and model real systems or phenomena. Concerning Kolmogorov measure, the answer is that it gives an idea on the computing power and storage capacity needed to process the models related to the original natural problem. Besides, as Kolmogorov measures are based on system disorder, biological versatility can be estimated.

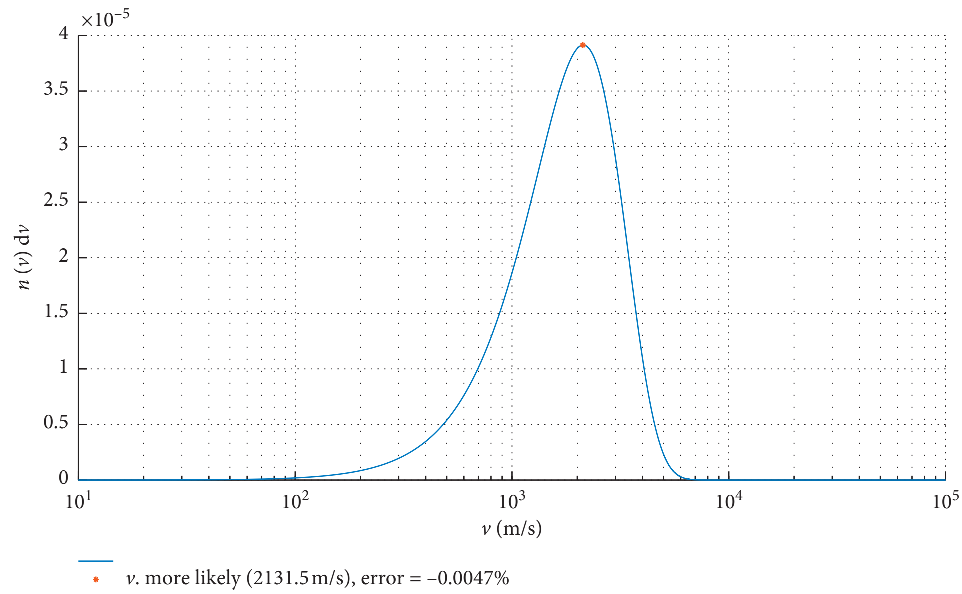


FIGURE 1: Maxwell–Boltzmann distribution for $T = 273$ K.

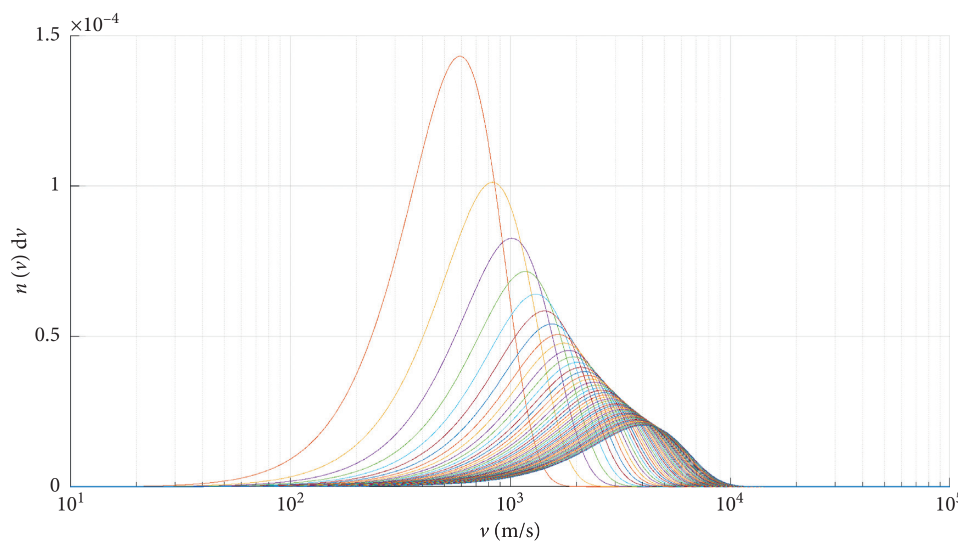


FIGURE 2: Maxwell–Boltzmann distributions for $T \in [20.41\,\text{K}, 1000\,\text{K}]$.

Another important point is that these three measures are defined considering discrete probability distributions with a finite domain, limiting their application. Some efforts to use them in biology and economy contexts [17, 18], providing ways to discretized data and obtaining complexity measures, are recently presented. Here, the idea is to apply the three measures to a well-known statistical physics problem and the continuous velocity distribution related to nuclear reactions to see if the discretizing process and complexity calculations produce useful interpretation about the phenomenon.

In the next section, the theoretical foundations are presented: Maxwell–Boltzmann velocity distribution of the thermal neutrons in a nuclear reactor and the three mentioned complexity measures. Then, a section of results with calculation of the measures for the known Maxwel–Boltzmann distribution, in function of the temperature, is presented. The analysis of these results is performed in the conclusion section.

2. Theoretical Foundations

2.1. Maxwell–Boltzmann Distribution. In a nuclear reactor, the fuel is composed of unstable atoms. They are used to generate a controlled nuclear reaction, in which the useful products are created. In a power reactor, part of the thermal energy generated in the nuclear reaction is converted into electrical energy, while high-energy neutrons are generated. These neutrons pass through a moderator, which reduces their kinetic energy [19].

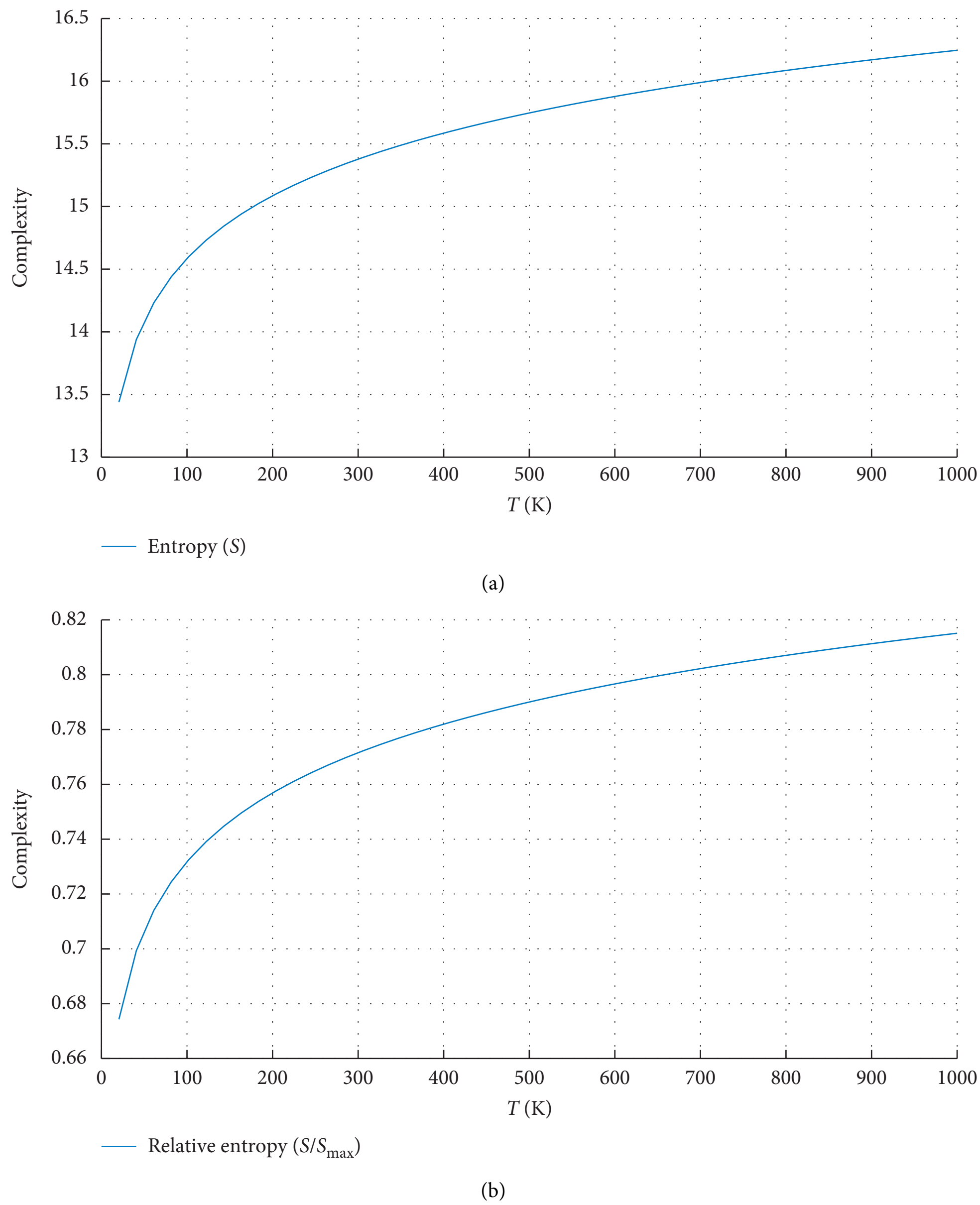


Figure 3: Thermal neutron Kolmogorov complexity. (a) Kolmogorov absolute complexity. (b) Kolmogorov normalized complexity.

The reason for that is to enlarge the cross section for the fission reaction. When neutrons loose enough energy to achieve thermodynamic equilibrium with the media where they are traveling in, they are called thermal neutrons. Because many nuclear reactors use a fluid as water to either refrigerate their nuclei or mediate neutrons generated in the reactions, the temperature of this media is of critical operational importance to determine the amount of heat that can be retrieved from the nucleus [20].

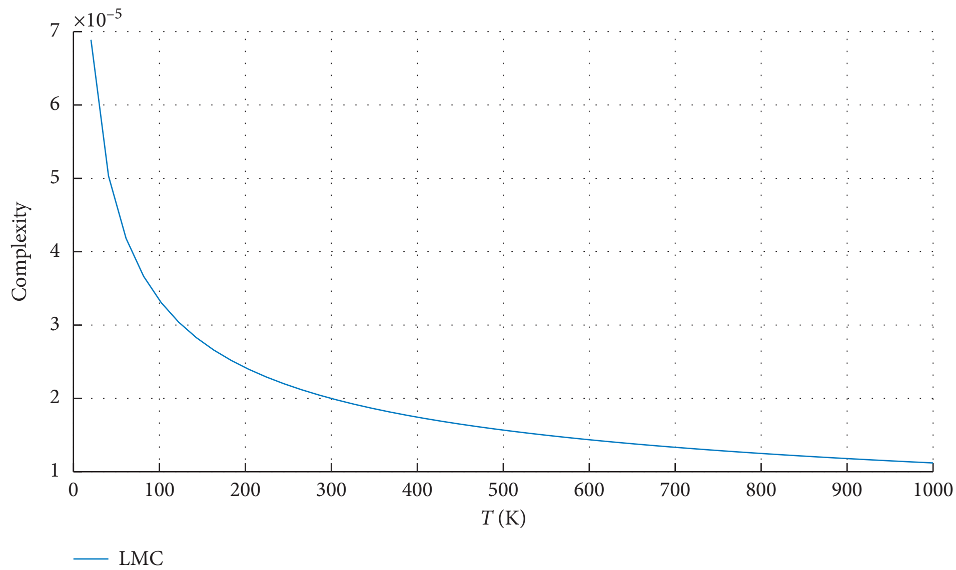
Besides, the thermal neutron velocity distribution is closely related to the media temperature obeying the Maxwell–Boltzmann law [19, 20], being an important statistical physics result. This distribution follows the equation

$$n(v)\mathrm{d}v = 4\pi n\left[\left(\frac{m}{2\pi K_B T}\right)^{3/2}\right]v^2 e^{-(mv^2/2K_B T)}\mathrm{d}v, \qquad (1)$$

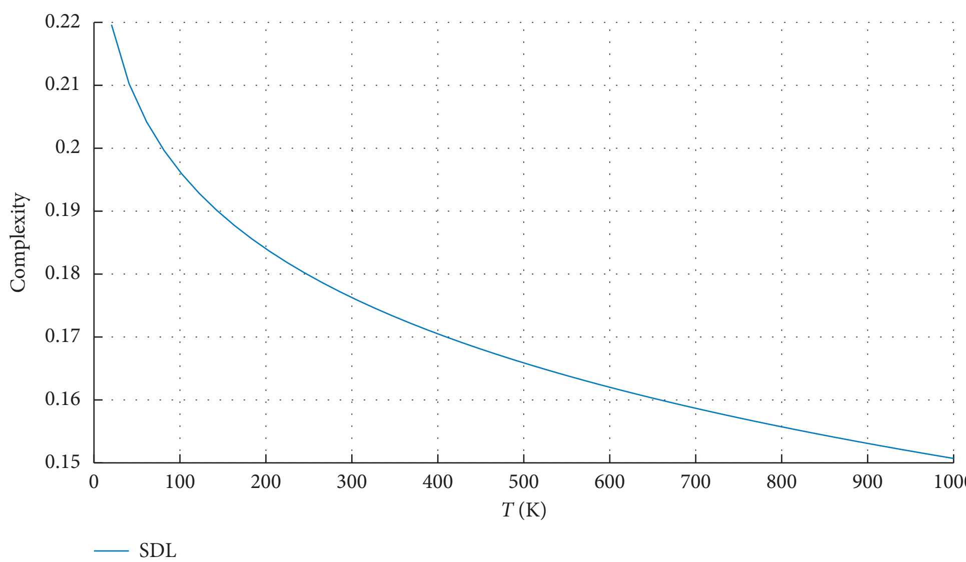
where $n(v)\mathrm{d}v$ is the number of neutrons with velocities between v and $v + \mathrm{d}v$; n is the number of neutrons in a unitary volume; m is the neutron mass (1.675×10^{-27} kg); K_B is the Boltzmann constant (1.380649×10^{-23} J/K); and T is the media temperature. Figure 1 shows the Maxwell–Boltzmann distribution for $T = 273\,\mathrm{K}$, giving the percentage of neutrons in each state, considering $n = 1$.

2.2. Complexity Measures. Here, the three complexity measures are briefly discussed and more detailed descriptions can be found in references [1, 9, 13]. The basic ideas of Kolmogorov, LMC, and SDL measures are based on the calculation of informational entropy.

For a discrete probability distribution composed of n possible states, each one with probability p_i, $i = 1, 2, \ldots, n$,



(a)



(b)

Figure 4: Thermal neutron complexities. (a) LMC complexity measure. (b) SDL complexity measure.

the informational entropy (E) associated with the distribution is given by [11]

$$E = -\sum_{i=1}^{n} p_i \log_2 p_i, \quad (2)$$

having (bit/state) as its unit.

2.2.1. Kolmogorov Complexity Measure. The first ideas about complexity measures were proposed by Kolmogorov, in the context of computational algorithms [1], whose complexity was related to the number of operations required by a Universal Turing Machine (UTM) to execute the algorithm. The main idea is that the minimum number of bits to write a code to run in a computer emulates a random process and is called Kolmogorov–Chaitin–Solomonoff complexity [21].

As the length of a code of a program can be interpreted as a string resulting from a free-compression algorithm, it makes the Kolmogorov–Chaitin–Solomonoff complexity closely related to the concept of information measure [1], presenting very similar results for the most of the algorithms [22, 23].

Considering this fact, the absolute Kolmogorov complexity is defined here as equal to the informational entropy E, whose maximum value, $E_{max} = \log_2 n$ occurs in the equiprobable case. As equiprobability of states corresponds to a completely disordered system, i.e., thermodynamic equilibrium, a normalized Kolmogorov complexity measure,

$\Delta \in [0, 1]$ can be defined as the system relative disorder, given by

$$\Delta = \frac{E}{E_{\max}}. \quad (3)$$

2.2.2. LMC Measure. Defining complexity measure in Kolmogorov's way gives an idea about necessary computation resources to describe a system or to perform a task and was useful to define versatility in biological phenomena [24]. Despite its utility, Kolmogorov measure was not considered adequate to measure complexity, because it gives only an idea about the state of disorder.

Considering that complex is a balance between order and disorder [8], López-Ruiz et al. proposed a measure taking order and disorder into account. The disorder was measured by the normalized Kolmogorov measure Δ, and the order (D) was measured by the quadratic deviation of the considered probability distribution from the uniform one; that is,

$$D = \frac{\sum_{i=1}^{n} \left(p_i - (1/n)\right)^2}{n}. \quad (4)$$

Consequently, the LMC (López-Ruiz et al.) complexity measure is defined by [9]

$$\mathrm{LMC} = \Delta \times D. \quad (5)$$

2.2.3. SDL Measure. Considering the same idea of the LMC measure, i.e., taking order and disorder into account, Shiner, Davison, and Landsberg simplified the calculation considering that order can be measured just as the complement of disorder and, consequently, proposed de SDL (Shiner et al.) measure [13]:

$$\mathrm{SDL} = \Delta \times (1 - \Delta). \quad (6)$$

It can be noticed that the measures of order (disequilibrium) are different for the two measures but defined in simple operational ways. For the sake of simplicity, improvements of these definitions considering Kullback–Liebler measure [25] are not considered.

3. Results

To apply the complexity measures to the Maxwell–Boltzmann statistical distribution and to show how they depend on the temperature (T), 49 distributions for $T \in [20.41\,\mathrm{K}, 1000\,\mathrm{K}]$ were generated as shown in Figure 2.

Then, for each temperature, the distribution was discretized taking $n = 1000$ uniformly sequential intervals $\Delta v = 0.1$ m/s between 10 m/s and 10,000 m/s and associating the probability given by $p \cdot \Delta v$ with each interval. Then, a discrete probability distribution for v was associated with each temperature.

Taking these distributions, informational entropies (E) can be calculated, with the results about how E, representing Kolmogorov absolute complexity, in (bit/state), depends on T shown in Figure 3(a). Based on the data obtained to build Figures 2 and 3(a), normalized Kolmogorov complexity was calculated, with the results about how Δ depends on temperature T shown in Figure 3(b).

As Figure 3 shows, Kolmogorov complexity of Maxwell–Boltzmann distribution increases with temperature, indicating that the thermal neutron set goes to a thermodynamic equilibrium.

To analyze how the thermal neutron system generates a complex system, considering the order-disorder balance, LMC and SDL complexity measures were calculated, and their dependence with temperature is shown in Figure 4.

4. Conclusions

Using complexity measures to the problem related to Maxwell–Boltzmann distributions gives some hints about the behavior of the thermal neutron set in a nuclear reactor:

(i) Kolmogorov measures have their values softly varying for a wide range of temperatures. However, above 600 K, the measures remain practically constants.

(ii) SDL measure indicates that complexity decreases with temperature, tending to 0.15, indicating that disorder surpasses order as temperature increases.

(iii) LMC measure results are similar to SDL, but in a smaller scale of values.

(iv) According to Figures 3 and 4, it be conjectured that $\lim_{T \longrightarrow \infty} \Delta = 1$ and $\lim_{T \longrightarrow \infty} \mathrm{LMC} = \lim_{T \longrightarrow \infty} \mathrm{SDL} = 0$. These values could be numerically reached increasing the number of discretization points.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this article.

Acknowledgments

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