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Complex Dynamical Systems and Mathematical Modelling

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Abstract
So-called "Complex Dynamical Systems" (that is, systems displaying complex behavior) do appear in condensed matter physics and chemistry, as well as, playing a fundamental role, in biological systems. They require a theoretical treatment in terms of "Mathematical Modelling", with statistical formalisms being of large relevance. We present here a feature-like article describing and discussing the question. It has emphasized the difficult question of presence of hidden constraints, and the introduction of nonstandard statistics arising in the realm of "Information Theory".

Keywords: *Information theory, statistical approach, hidden constraints, nonstandard statistics*

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INTRODUCTION

More than 40 years ago, Montroll and Shlesinger wrote that "in the world of investigation of complex phenomena that require statistical modelling and interpretation several competing styles have been emerging, each with its own champions" [1]. The study of certain physical-chemical systems we may face difficulties when handling situations involving fractal-like structures, correlations (spatial and temporal) with some type of scaling, turbulent or chaotic motion, small size (nanometric scale) systems, which eventually involve a low number of degrees of freedom, and so on. It is in these situations that we are faced with the existence of "hidden constraints" to which we do not have access.

The interest on the study of such kind of complex physical systems has been recently enhanced as a consequence that they are part of electronic and opto-electronic devices of the nowadays advanced technologies, and also in technological/industrial areas involving the use of disordered systems, polymeric solutions and materials, ion-conducting glasses, the case of micro-batteries and others. Also it is of high relevance, the question of the emerging and largely expanding systems biology, involving complexity, self-organization and information theory [2].

Theory of dynamical systems is considered to be pioneered by Bertalanffy who wrote that "If someone were to analyze current notions and fashionable catchwords, he would find 'systems' high on the list. The concept has permeated all fields of science and penetrated into popular thinking, jargon, and mass media" in the introduction of his 1967 book which was a compilation of his writings, the first contributions dating from the to mid-1930's [3].

Mathematical modelling is nowadays an integral part of current research in biology, particularly in molecular cell biology and systems biology in general. Dynamical investigations of biological systems place them in a common conceptual framework, trying to indicate how this framework can be used to formulate and solve many of the important and perplexing problems of biology, particularly those dealing with regulation and control in the broadest sense [4].

In particular we may mention cellular modelling, a particularly challenging task of systems biology and mathematical biology; multicellular organism simulation; protein folding prediction of their three-dimensional structure from its amino acid sequence; brain model down to the molecular level; model of the immune system; virtual liver, a project to produce a dynamic mathematical model representing human liver; ecological models, i.e., mathematical representation of ecosystems; models in ecotoxicology, that is, simulation and prediction of effects produced by toxic compounds in the environment; modelling of infectious diseases, to predict the likely outcome of an epidemic; and so on and so forth.

Another important topic involving mathematical modelling is the one of spontaneous generation of spatial patterns, originated with Turing [5]. It has been said that Turing was the same man who helped discover the German high command's ultra-secret for encrypting codes during World War II and the same man laid loud the basis for modern computers with his analysis of the logical requirements for algorithms in his Turing machine, and also formulated a fundamental idea concerning the onset of patterns in organism [6].

In what follows, we do here emphasize the aspects of statistical approaches, and we close this introduction calling the attention to the description of modeling biological systems in http://en.wikipedia.org/wiki/modelling_biological_systems, where are given extensive references of published research.

THE STATISTICAL APPROACH

As stated at the beginning of the introduction, statistics plays a fundamental role in the area of mathematical modeling of systems, particularly, as noticed, in condensed matter physics [7] and biology [8].

Complexity is present in many cases (self-organization is the rule in biological systems) involving in multiples occasions the difficulty of having to face the presence of hidden constraints, that is, not to have access to information which is quite relevant to the proper description of properties of the system. The question involves the fact that the researcher faces difficulties in satisfying [9] Fisher's criteria of efficiency and sufficiency in the conventional approach to the well-established, physically and logically sound Boltzmann-Gibbs statistics ("The criterion of efficiency is satisfied by those statistics which, derived from large samples, tend to a normal distribution with the least possible standard deviation" and, "A statistics satisfies the criterion of sufficiency when no other statistics which can be calculated from the same sample provides any additional information as the value of the parameter to be estimated", which for the purpose of statistical mechanics is to be taken as the existence of an incomplete description of the physical situation in hands [10]). In statistical mechanics the question typically consists in that one needs to confront some impairment on how to correctly include the presence of large fluctuations (and eventually higher-order variances) and to account for the relevant and proper characteristics of the system, implying in lack of efficiency and sufficiency, respectively. As a consequence, in an attempt to assuage these difficulties, and thus allowing to improve the predictions, one may resort to statistical approaches other than the consistent and, say, canonical one of Boltzmann-Gibbs.

Among existing approaches we can mention:

1) The one used by Landsberg showing that functional properties of the (informational) entropies give, in fact, origin to different types of unusual thermo-statistics, and raise the question of how to select a "proper" one, that is, some better than others? [11].
2) For dcades it has been in use in Lèvy Statistics, introducing modified non-Gaussian distributions, which has been applied to a variety of problems, and recently it had a revival with its application to the study of chaotic dynamics (see for example Refs. [1, 12, 13]).
3) The approach of Ebeling who has addressed the question of the statistical treatment of a class of systems that are in some sense "anomalous" [14, 15]. They contain those in nature and society which

are determined by its total history. Usually the given examples are the evolution of the Universe and of our planet, phenomena at the biological, ecological, climatic, social levels, etc. The approach consists into introducing conditional probabilities in the context of Boltzmann-Gibbs formalism in Shannon-Jaynes approach, leading to a thermo-statistics appropriate for describing complex processes with long ranging memory and including correlations [14–16].

4) The so-called "Super-Statistics" developed by Beck and Cohen for non-equilibrium systems with complex dynamics in stationary states with large fluctuations on long-time scales [17].
5) The generally called "Non-Extensive Thermo-Statistics", based on Havrda-Charvat approach [18], which applied to several cases is described in the Conference Proceedings of Abe *et al.* [19].
6) "Renyi approach" [20, 21] has been introduced in the scientific literature, as noticed in Ref. [22], with, for example, Grassberger and Procaccia [23, 24] using it in a modified form as a valuable method for characterizing experimental chaotic signals.
7) Jizba and Arimitzu have presented an extensive analysis of it in a paper called "The world according to Renyi", where they show that making extreme Shannon's entropy on a multi-fractal is equivalent to directly making extreme Renyi's entropy without invoking the multi-fractal structure explicitly [25].
8) Sharma-Mittal approach [26] or better to say a variation of it (called Kappa or Deformational Statistics), was used by Vasyliunas in problem of astrophysical plasma [27] and by Kanadiakis in the case of relativistic systems [28].

We recall that in statistical mechanics, the probability distribution (statistical operator), usually derived from heuristic arguments, can also be derived from an extreme-principle formalism once it made connection with information theory [29–31]. It consists into making a maximum, subjected to certain constraints, a functional (super-operator). Such quantity, first introduced in Shannon's theory of communication, can be referred to as "measure of uncertainty of information" [32]. It has also been called statistical measure and entropy, with the understanding that it is "information-theoretic entropy". It is worth to emphasize, in view of some confusion that has recently pervaded the scientific literature that *the different possible information theoretic entropies are not to be interpreted as the thermodynamic entropy of the physical system*. Cox has noticed that the meaning of such entropies is not the same in all respects as that of anything which has a familiar name in common use, and it is therefore impossible to give a simple verbal description of it, which is, at the same time, an accurate definition [33]. Jaynes has also commented that it is an unfortunate terminology, and a major occupational disease in that *there exists a persistent failure to distinguished between the informational entropy, which is a property of any probability distribution, and the experimental entropy of thermodynamics which is instead a property of a thermodynamic state: Many research papers are flawed fatally by authors' failure to distinguish between these entirely different things* (emphasis is ours), and in consequence proving nonsense results [34].

Gibbs-Boltzmann-Shannon information-theoretic entropy (Kullback-Leibler measure in Information Theory [35]) is given by:

$$S_{\mathrm{GBS}}(t) = \mathrm{Tr}\{\mathrm{R}(t) \ln \mathrm{R}(t)\} \quad (1)$$

with $\mathrm{R}(t)$ being the statistical operator for the corresponding Gibbs' ensemble. The derivation of the statistical operator $\mathrm{R}(t)$ has been done using various consistency arguments, (see for example the review article by Balian and Balazs [36]). Among them we can highlight the one based on heuristic arguments (as it is usual in the textbooks for the case of equilibrium, and for non-equilibrium systems, see for example [37, 38]), and the one using a extremal-principle approach consisting in maximizing $S_{\mathrm{GBS}}(t)$ subjected to constraints (the so-called MaxEnt formalism) [29, 30].

Concerning statistical mechanics of many-body systems, it may be noticed that it has a long and successful history. The introduction of the concept of probability in physics originated mainly from the fundamental essay of Laplace [39], who incorporated and extended some earlier seminal ideas (see a historical review in Ref. [40]). As well known, statistical mechanics attained the status of a well-established discipline at the hands of Maxwell, Boltzmann, Gibbs, and others, and went through some steps related to changes, not in its fundamental structure, but just on the substrate provided by microscopic mechanics. Its application to the case of systems in equilibrium proceeded rapidly and with exceptional success; equilibrium statistical mechanics gave, starting from the microscopic level, foundations to thermostatics, and the possibility to build a response function theory. Applications to non-equilibrium systems began, mainly, with the case of local equilibrium in the linear regime following the pioneering work of Onsager [41, 42].

For systems arbitrarily deviated from equilibrium and governed by nonlinear kinetic laws, the derivation of an ensemble-like formalism proceeded at a slower pace than in the case of equilibrium, and somewhat cautiously, with a long list of distinguished scientists contributing to such development. It can be noticed that statistical mechanics gained in the 1950s an alternative approach sustained on the bases of information theory [30, 37, 38, 40, 43–47]. It invoked the ideas of information theory accompanied with ideas of scientific inference [48, 49], and a extremal-principle formalism (the latter being Jaynes' principle of maximization of informational uncertainty, also referred-to as informational entropy, MaxEnt for short), compounding from such point of view a theory dubbed *Predictive Statistical Mechanics* [30, 31, 40, 43–47]. It should be noticed that this is not a new paradigm in statistical physics, but a quite useful and practical extremum-principle which codifies the derivation of probability distributions, which are usually obtained by either heuristic approaches or projection operator techniques [29, 50, 51]. It is particularly advantageous for building non-equilibrium statistical ensembles allowing for the systematization of the relevant work on the subject that renowned scientists provided along the past century, as described by Luzzi [29].

Moreover, it has been noticed that MaxEnt is not a physical principle in the proper sense, and should be carefully distinguished from the "entropy maximum principle" of thermodynamics. The latter is not a rule of inference but a condition of thermodynamic equilibrium [52]. MaxEnt, apparently first proposed by Elssasser [53], was analyzed in depth, largely systematized and extended by Jaynes, who proposed it as an extension of the principle of insufficient reason in Logic [44–46]. It has been claimed that MaxEnt is singled out as a unique method of statistical inference that agrees with certain compelling consistency requirements.

The point has been critically reviewed by Uffink [52]. Moreover, Landauer has argued that "advocacy of MaxEnt is perpetuated by selective decision making in the generation of papers [...] MaxEnt is likely to be sound, but often it is dreadfully difficult to understand what the constraints are" [54]. Bunge stated that "when confronted with a random or seemingly random process, one attempts to build a probabilistic model that could be tested against empirical data, no randomness, no probability" [55]. Moreover, as Poincare pointed out long ago, talk of probability involves some knowledge; it is not a substitute for ignorance (and Bunge adds, not correctly, in what refers to the statistical mechanics we are discussing here, that) "this is not how the Bayesian or a personal view, the matter when confronted with ignorance or uncertainty, they use probability or rather their own version of it. This allows them to assign prior probabilities to facts and propositions in an arbitrary manner (again, this is not the case in MaxEnt-based Non-Equilibrium Statistical Ensemble Formalism), which is a way of passing off mere intuition, hunch, or guess for scientific hypothesis [...]; it is all a game of belief rather than knowledge". Sometimes arguments against MaxEnt in terms of playing dices have been advanced. To this, it must be recalled that the question we are addressing here does not deal with gambling, but with many-body theory, that is, we deal with systems with very many degrees of freedom, and then is necessary to have in mind the distinction between interpretations in terms of microscopic and macroscopic variables.

The spirit of the formalism is to make use of the restricted knowledge available, but without introducing any spurious one. Quoting Laplace, "the curve described by a molecule of air or of vapor is following a rule as certainly as the orbits of the planets; the only difference between the two is our ignorance [39]. Probability is related, in part to this ignorance, in part to our knowledge". Also, as pointed out by Bricmont, "the part 'due to our ignorance' is simply that we use probabilistic reasoning; if we were omniscient, it would not be needed (but the averages would remain what they are, of course) [56]. The part 'due to our knowledge' is what makes reasoning work [...]. But this is the way things are; our knowledge is incomplete, and we have to live with that. Nevertheless, probabilistic reasoning is extraordinarily successful in practice, but, when it works, this is due to our (partial) knowledge. It would be wrong to attribute any constructive role to our ignorance. And it is also erroneous to assume that the system must be somehow indeterminate when we apply probabilistic reasoning to it." [57]. It has been noticed that to derive the behavior of the macroscopic state of the system from partial knowledge has been already present in the original brilliant work of Gibbs.

Heisenberg wrote "Gibbs was the first to introduce a physical concept which can only be applied to an object when our knowledge of the object is incomplete" [58]. Furthermore, it can be considered that the dismissal of a theoretical approach in physics cannot (and should not) be done on the basis of general verbal arguments, which may or may not be sensible, but which need be strongly founded on the scientific method. In other words, the merits, or rather demerits, of a theory reside in establishing its domain in of validity (see for example Refs. [59, 60]), when tested against the experimental results it predicts.

This point has recently been forcefully stressed by Hawkings [61]. On the particular case of the extremum-principle approach in Jaynes style (as an alternative way [38], e.g., the heuristic one [62] for building the Non-Equilibrium Statistical Ensemble Formalism), Sklar has summarized that Jaynes firstly suggested that equilibrium statistical mechanics can be viewed as a special case of the general program of systematic inductive reasoning, and that, from this point of view, the probability distributions introduced into statistical mechanics have their bases not so much in an empirical investigation of occurrences in the world, but, instead in a general procedure for determining appropriate a priori subjective probabilities in a systematic way [63].

Additional analyses are present in the work of Fraassen, where it is discussed the possibility of alternative rules of construction of generalized (information-theoretic) entropy expressions containing a free continuous parameter (so-called Renyi entropies), that is, of the type of those considered here. Uffink noticed that it seems that more research would be needed to assess their performance in concrete cases and in general [64–66].

Moreover, in an article properly titled 'Entropies Galore!' [11], Peter Landsberg has called the attention to the fact that, very-many of these information-theoretic entropies can be proposed [67].

The informational-based approach has been quite successful in its application to the cases of equilibrium and near equilibrium conditions [37, 38, 43, 44], and in the last decades has been, and is being, also applied to the construction of a generalized ensemble theory for systems arbitrarily away from equilibrium [29, 50, 51, 68–71]. The non-equilibrium statistical ensemble formalism (NESEF) provides mechanical-statistical foundations to irreversible thermodynamics (in the form of Informational Statistical Thermodynamics, ITE for short [72–75]), a nonlinear quantum kinetic theory [29, 50, 51, 76–79] and a response function theory [29, 80] of a large scope for dealing with many-body systems arbitrarily far removed from equilibrium. NESEF has been applied with success to the study of a number of non-equilibrium situations in the physics of semiconductors (see for example the review article of Ref. [7]) and polymers [81], as well as to studies of complex behavior of boson systems in, for example, biopolymers (e.g. Ref. [8]) and phonon systems [82]). It can also be noticed that the NESEF-based nonlinear quantum kinetic theory provides, as particular limiting cases, far-reaching generalizations of Boltzmann [83], and Mori equations [84], together with statistical foundations for mesoscopic irreversible thermodynamics [85, 86], and a higher-order hydrodynamics [86–90].

NESEF is built on the bases of heuristic standard arguments (see for example Ref. [62]), or within the scope of the extremum-principle method based on the maximization of the information-theoretic-entropy of Shannon-Jaynes approach in Boltzmann-Gibbs statistics given in Eq. (1), that is, the average of minus the logarithm of the time-dependent, i.e., depending on the irreversible evolution of the macroscopic state of the system 'non-equilibrium statistical operator'. We again emphasize that information-theoretic-entropy is in fact the quantity of uncertainty of information, and has the role of a generating functional for the derivation of probability distributions (for tackling problems in communication theory, physics, mathematical economics, and so on). There is one and only one situation when Shannon-Jaynes informational-entropy coincides with the physical entropy of Clausius in thermodynamics, namely, the case of strict equilibrium [11, 91].

We have already called the attention to the classical and fundamental paper of 1922 by Fisher, titled "On the Mathematical Foundations of Theoretical Statistics", where the basic criteria that a statistics should satisfy in order to provide valuable results are presented. We reiterate that in present day statistical mechanics in physics, two of them are of major relevance, namely the criterion of efficiency and the criterion of sufficiency already described. This is so because of particular constraints which are present, for example, in physical situations involving small systems, where on the one hand the number of degrees of freedom entering in the statistics may be small, and on the other hand structures, including boundary conditions of a fractal-like character which strongly influence the properties of the system, are present. Such facts make it difficult to introduce sufficient information for deriving a proper Boltzmann-Gibbs probability distribution, and we may mention the examples of nanotechnology, nanobiophysics, quantum dots and nanometric hetero-structures in semiconductor devices, one-molecule transistors, fractal-electrodes in microbatteries, and so on. Other case where the sufficiency criterion is difficult to satisfy is the one of large systems of fluids whose hydrodynamic motion is beyond the domain of validity of the classical standard approach. It is then required the use of a nonlinear higher-order hydrodynamics, eventually including correlations and other variances (a typical example is the case of turbulent motion). This has an analogy in the treatment of biosystems.

CONCLUSIONS

The so-called *Complex Dynamical Systems* (a short for systems displaying complex behavior) are systems with unexpected emerging properties which are the result of synergetic processes of their components, whose treatment largely depends on mathematical modelling and the accompanying statistical approaches.

We have presented a description of the question with emphasis on the associated statistical approach. Particular attention has been done on the basis of *Information Theory in a Shannon-Jaynes approach* in the spirit of Jeffreys' scientific inference proposal.

Some attention has also been given to the difficulties brought about by the inconvenience of the presence of *hidden constraints*. Some comments are included on the question of the use of nonstandard statistics, particularly the Renyi one.

It has been noticed in the main text that the foundations of statistical mechanics on information theory have been quite successful in its applications to the situations of equilibrium and near equilibrium conditions, and is being used in the construction of a generalized ensemble theory for systems arbitrarily away from equilibrium involving relaxation processes ultra-rapid in time (pico- and femto-second scales) and in ultra-small regions (nanometer scales).

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