Physica A 418 (2015) 94–104

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

About the role of chaos and coarse graining in statistical mechanics

G. Falasco [a], G. Saggiorato [b,*], A. Vulpiani [c]

[a] *Institut für Theoretische Physik, Universität Leipzig, Postfach 100920, Leipzig 04009, Germany*
[b] *Theoretical Soft Matter and Biophysics, Institute of Complex Systems and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany*
[c] *Department of Physics, University of Roma "Sapienza", P.le A. Moro 2, I-00185 Roma, Italy*

HIGHLIGHTS

- We discuss the role of ergodicity and chaos for the validity of statistical laws.
- We explore the basic aspects of chaotic systems on systems composed of a huge number of particles.
- We emphasize on the finite-resolution aspects.

ARTICLE INFO

Article history:
Available online 2 June 2014

Keywords:
Ergodic theory
Chaos
Entropy
Finite-resolution effects

ABSTRACT

We discuss the role of ergodicity and chaos for the validity of statistical laws. In particular we explore the basic aspects of chaotic systems (with emphasis on the finite-resolution) on systems composed of a huge number of particles.

1. Introduction

Statistical mechanics was founded by Maxwell, Boltzmann and Gibbs to account for the thermodynamics of macroscopic bodies, i.e. systems with a very large number of particles, starting from the microscopic interactions. The typical claim is that statistical mechanics works without very precise requirements on the underlying dynamics (except for the assumption of ergodicity). With the discovery of deterministic chaos it became clear that statistical approaches may also be unavoidable and useful in systems with few degrees of freedom. However, even after many years there is no general agreement among the experts about the fundamental ingredients for the validity of statistical mechanics.

The wide spectrum of positions ranges from the belief of Landau and Khinchin in the main role of the many degrees of freedom and the (almost) complete irrelevance of dynamical properties, in particular ergodicity, to the opinion of those, for example Prigogine and his school, who consider chaos as the basic ingredient.

For almost all practical purposes one can say that the whole subject of statistical mechanics consists of the evaluation of a few suitable quantities (for example, the partition function, free energy, correlation functions). The ergodic problem is often forgotten and the (so-called) Gibbs approach is accepted because "it works". Such a point of view cannot be satisfactory, at least if one believes that it is not less important to understand the foundation of such a complex issue than to calculate useful quantities.

---

* Corresponding author. Tel.: +49 2461613913.
E-mail address: g.saggiorato@fz-juelich.de (G. Saggiorato).

http://dx.doi.org/10.1016/j.physa.2014.05.030

The present paper is meant to serve as a short informal introduction to the problem of the connection between dynamical behavior (mainly ergodicity and chaos) and statistical laws.

This contribution has been written by G.S. and G.F from the lectures delivered by A.V.

2. The bridge to statistical mechanics

Before moving on to a more technical discussion we want to elucidate the pivotal role played by ergodicity in passing from a mechanical to a statistical description of a macroscopic system. Let us consider an isolated system of N particles. Denoting by $\boldsymbol{q}_i$ and $\boldsymbol{p}_i$ the position and momentum vectors of the ith particle, the state of the system at time t is described by the vector $\boldsymbol{x}(t) = (\boldsymbol{q}_1(t), \dots, \boldsymbol{q}_N(t), \boldsymbol{p}_1(t), \dots, \boldsymbol{p}_N(t))$ in a $6N$-dimensional phase space. The evolution law is given by Hamilton's equations. Given a physical observable $A(\boldsymbol{x})$, its time average over a period T is defined by:

$$\overline{A}^T(\boldsymbol{x}(0)) = \frac{1}{T}\int_0^T A(\boldsymbol{x}(t))\mathrm{d}t. \tag{1}$$

In general (1) is a function of the averaging time T and of the initial conditions $\boldsymbol{x}(0)$. We assume that $\overline{A}^T$ is the result of an experimental measurement, i.e. is performed on a macroscopic time T. Therefore, since T is much larger than the microscopic dynamics time scale over which the molecular changes occur, the formal limit $T \to \infty$ can be considered. We say that the ergodic hypothesis is satisfied if the time average

$$\overline{A} \equiv \lim_{T\to\infty} \frac{1}{T}\int_0^T A(\boldsymbol{x}(t))\mathrm{d}t, \tag{2}$$

is a function of the energy only, independent of the initial conditions. If it is the case, the time average (2) can be replaced by the probability average

$$\overline{A} = \int \rho_{\mathrm{mc}}(\boldsymbol{x})A(\boldsymbol{x})\mathrm{d}\boldsymbol{x} \equiv \langle A\rangle, \tag{3}$$

where $\rho_{\mathrm{mc}}(\boldsymbol{x})$ is the micro-canonical probability density function, defined constant over a constant energy surface. The validity of (3) constitutes the main question of the ergodic problem. In the following we address the issue of identifying the conditions under which a dynamical system is ergodic. It will soon be clear that mathematical ergodicity is extremely difficult to be asserted and, in fact, weaker properties can be required to physical systems.

Let us wonder about the basic question of the foundation of the statistical mechanics: why do the time averages of the microscopic properties of a system of particles describe the thermodynamic properties of the object composed of those particles? The microscopic system, in fact, consists of a myriad of mechanical parameters, such as the particles, energy and momentum, while thermodynamics consists of just a few measurable quantities, like temperature and pressure. The corresponding diversity of fundamental terminology, qualifies the reduction of thermodynamics to mechanics as "heterogeneous" reduction [1], a condition which may prevent the logical derivation of the former theory from the latter. For such a problem the typical approach of the philosophy of science is to require the existence of relations between the terms of the mechanics and elements of the vocabulary of thermodynamics. Such bridge law must reflect a kind of identity between the objects of study of the two theories [1]. The bridge law which associates thermodynamics with the classical mechanics of atoms was proposed by Boltzmann and it is engraved in his tomb stone:

$$S = k\log W. \tag{4}$$

This celebrated relation connects the thermodynamic entropy S of an object in the macroscopic state X, to the volume W of all microstates correspond to the same X. For example, considering the macrostate X corresponding to a given energy E, one typically considers the energy shell $E - \delta E \le H(\{\mathbf{q}_n\}, \{\mathbf{p}_n\}) < E$, with small δE, and obtains:

$$W = \int_{E-\delta E\le H(\mathbf{q},\mathbf{p})<E} \mathrm{d}\mathbf{q}_1 \dots \mathrm{d}\mathbf{q}_N \mathrm{d}\mathbf{p}_1 \dots \mathrm{d}\mathbf{p}_N.$$

The micro-canonical probability distribution is constant (equal to $1/W$) in the energy shell and zero otherwise. Eq. (4) qualifies as a bridge law, because S is a thermodynamic quantity, while W is a microscopic entity. Once it has been introduced, further mechanical properties of our description of the microscopic dynamics may be related to as many other thermodynamic quantities, thus bridging the gap between micro- and macro-descriptions.

3. Some general considerations about ergodicity

Here we introduce the notion of dynamical system:

Definition (*Dynamical System*)**.** A deterministic dynamical system is described by the triplet (Ω, S^t, μ), where:

- Ω is the phase space containing the system state vector $\boldsymbol{x}$;
- S^t is the evolution operator: $\boldsymbol{x}(t) = S^t\boldsymbol{x}(0)$;
- μ is a measure invariant under the evolution S^t, i.e. $\mu(G) = \mu(S^{-t}G)$ for all $G \subset \Omega$.