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Patrizia Castiglione, Massimo Falcioni, Annick Lesne and Angelo Vulpiani
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CHAOS AND COARSE GRAINING IN STATISTICAL MECHANICS

While statistical mechanics can describe the equilibrium state of systems with many degrees of freedom, and dynamical systems can explain the irregular evolution of systems with few degrees of freedom, new tools are needed to study the evolution of systems with many degrees of freedom. This book presents the basic aspects of chaotic systems, with emphasis on systems composed of a huge number of particles.

The first part of the book introduces the basic concepts of chaotic dynamics. The book then moves on to explore the role of ergodicity and chaos for the validity of statistical laws. The last part of the book is devoted to the treatment of problems characterized by the presence of more than one significant scale. In addition, the authors also discuss the relevance that many degrees of freedom, coarse-graining procedure, and instability mechanisms, have in justifying a statistical description of macroscopic bodies. The book introduces the tools to characterize the non-asymptotic behaviors of chaotic systems. This text will be of interest to researchers and graduate students in statistical mechanics and chaos.

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Preface

Statistical Mechanics has been founded during the XIX-th century by the seminal work of Maxwell, Boltzmann and Gibbs, with the main aim to explain the properties of macroscopic systems from the atomistic point of view. Accordingly, from the very beginning, starting from the Boltzmann's ergodic hypothesis, a basic question was the connection between the dynamics and the statistical properties. This is a rather difficult task and, in spite of the mathematical progress, by Birkhoff and von Neumann, basically ergodic theory had a marginal relevance in the development of the statistical mechanics (at least in the physics community). Partially this was due to a misinterpretation of a result of Fermi[1] and a widely spreaded opinion (based also on the belief of influential scientists as Landau) on the key role of the many degrees of freedom and the practical irrelevance of ergodicity. This point of view found a mathematical support on some results by Khinchin who was able to show that, in systems with a huge number of particles, statistical mechanics works (independently of the ergodicity) just because, on the constant energy surface, the most meaningful physical observables are nearly constant, apart from regions of very small measure,

On the other hand the discovery of the deterministic chaos (from the anticipating work of Poincaré to the contributions, in the second half of the XX-th century, by Chirikov, Hénon, Lorenz and Ruelle, to cite just the most famous) beyond its undoubted relevance for many natural phenomena, showed how the typical statistical features observed in systems with many degrees of freedom, can be generated also by the presence of deterministic chaos in simple systems. For example low dimensional models can emulate spatially extended dynamics modelling transport and conduction processes.

[1] A theorem about non integrable Hamiltonian systems with N degrees of freedom assures the non existence of smooth invariant surfaces of dimension $2N - 2$; from this result Fermi (erroneously) concluded that generic Hamiltonian systems are ergodic.

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Surely the rediscovery of deterministic chaos has revitalized investigations on the foundation of Statistical Mechanics forcing the scientists to reconsider the connection between statistical properties and dynamics. However, even after many years, there is not a consensus on the basic conditions which should ensure the validity of the statistical mechanics. Roughly speaking the two extreme positions are the "traditional" one, for which the main ingredient is the presence of many degrees of freedom and the "innovative" one which considers chaos a crucial requirement to develop a statistical approach.

It is unnecessary to stress the role of simplified models and numerical simulation. Because of technical difficulties in the treatment of any realistic system, the numerical study of simple models is essential. One of the first numerical experiments was the celebrated paper *Studies of non-linear problems* by Fermi, Pasta and Ulam, that showed that the ergodic problem was still far from being solved; and pointed out the necessity of using numerical simulation as a research tool complementary to analytical studies.

The main aim of this book is to show how, for understanding the conceptual aspects of the statistical mechanics, one has to combine concepts and techniques developed in the context of the dynamical systems with statistical approaches able to describe systems with many degrees of freedom. We discuss with particular emphasis the relevance of non asymptotic quantities, *e.g* ϵ-entropy, and the role of pseudochaotic systems, *i.e.* non chaotic systems with a non trivial behaviour.

We do not pretend to write a treatise on dynamical systems or statistical mechanics, however we tried to make the book as self-contained as possible.

The book is divided into three parts:

Part I : **Deterministic chaos and complexity** (Chapters 1, 2 and 3)
Part II : **Foundation of equilibrium and non equilibrium statistical mechanics** (Chapters 4, 5 and 6)
Part III : **Effective equations, multiscale and renormalization group** (Chapters 7 and 8)

In the first part we start introducing the basic concepts and ideas on chaotic dynamics. There exist well established ways to define the complexity of a temporal evolution, in terms of either Lyapunov exponents (LE) or Kolmogorov-Sinai (KS) entropy. This approach has been rather successful in deterministic low dimensional systems. On the other hand in high dimensional systems, as well as in low dimensional cases without a unique characteristic time some interesting features cannot be captured by LE or KS entropy. The basic reason of this weakness is that these quantities are properly defined only in specific asymptotic limits, that are: very long times and arbitrary accuracy. On the contrary in realistic situations one has to deal with finite accuracy and finite time, so it is important to take into account these limitations. For instance relaxing the limit of arbitrary high accuracy, one can

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introduce suitable tools, such as the Finite Size Lyapunov Exponent (FSLE) and the ϵ-entropy.

An analysis in terms of *FSLE* and ϵ-entropy allows for the characterization of non trivial systems in situations far from asymptotic (*i.e.* finite time and finite observational resolution). In particular we discuss the utility of ϵ-entropy and FSLE for a pragmatic classification of signals, and the use of chaotic systems in the generation of sequences of (pseudo) random numbers.

The second part discusses the role of ergodicity and chaos for the validity of statistical laws. Detailed numerical studies show in a clear way that for high dimensional Hamiltonian systems chaos is not a fundamental ingredient for the validity of the equilibrium statistical mechanics. Therefore the point of view that good statistical properties need chaos is unnecessarily demanding: even in the absence of chaos, one can have (according to Khichin ideas) a good agreement between the time averages and the predictions by the equilibrium statistical mechanics.

About the problem of the irreversibility of macroscopic processes it seems to us that Boltzmann was basically able to understand the essence of mechanism of the Second Law. The possible presence of chaos plays a minor role while the relevant aspects are the large number of degrees of freedom, and the selection of "good" initial conditions in such a way that the molecular chaos hypothesis is satisfied. With such assumptions one can eliminate the fluctuations in the time behaviour of $\mathcal{H}(t)$ vs t and therefore the classical objections by Loschmidt and Zermelo are overcome. Exact mathematical results have shown that the original intuitions of Boltzmann were correct.

Usually one deals with the behaviour of single macroscopic systems, and indeed thermodynamics, as a physical theory, has been developed to describe the properties of single systems, made of many microscopic, interacting parts. Thus it seems to us that it is quite fair to conclude that statistical ensembles are just useful mathematical tools. The study of a system made of many weakly coupled subsystems evidences the objective nature of the growing in time of the Boltzmann entropy, *i.e.* its independence from the coarse graining resolution, as far as it is small enough.

There is a rather strong evidence that chaos (in the technical sense of the existence of a positive Lyapunov exponent) is not a necessary ingredient for the validity of the statistical mechanics laws as diffusion and conduction. Numerical results show that the basic elements are: an instability mechanism, able to induce a particle dispersion at small scales, and the suppression of periodic orbits, to allow for a diffusion at large scale. In chaotic systems the instability mechanism is nothing but the sensitivity to the initial condition; however also in systems with zero maximal Lyapunov exponent finite-size instability mechanisms can exist.

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The last part is devoted to the treatment of problems characterized by the presence of more than one significant scale, *i.e.* with a variety of degrees of freedom with different time scales. For this class of systems it is necessary, both practically and conceptually, to treat the "slow dynamics" in terms of effective equations. These equations are able to catch some general features and to evidence dominant ingredients which can remain hidden in the detailed description.

We discuss some general aspects of the multiple-scale method and its connection with other important issues as the renormalization group. We see at work, in some simple cases,the basic tools necessary for the study of phenomena as diffusion and mesoscopic description of non-equilibrium statistical mechanics. In multiscale analysis one replaces the original evolution equation with an effective one which is valid at very large time (or at large spatial distance). As an example we can mention the asymptotic behaviour of the transport problem as described by a Fick's equation containing the eddy diffusion coefficients to take into account the inhomogeneity due to the advection field in the original problem.

This book is not an updated text of the most recent progresses in all the fields of statistical physics (in particular those regarding non equilibrium stationary states). Since we want to limit the treatment to some basic aspects, we do not discuss those results like fluctuations theorems which, for the technical aspects would almost deserve another and different book. Of course the selection of issues in this book reflects our scientific interest during the last years. We would like to express our thanks for inspiration, collaboration and correspondence to E. Aurell, L. Biferale, G. Boffetta, F. Cecconi, A. Celani, M. Cencini, E. Charpentier, P. Collet, A. Crisanti, D. del-Castillo-Negrete, P. Grassberger, C. Gruber, S. Isola, M.H. Jensen, K. Kaneko, H. Kantz, G. Lacorata, M. Laguës, R. Livi, V. Loreto, G. Mantica, U. Marini Bettolo Marconi, A. Mazzino, P. Muratore Ginanneschi, E. Olbrich, G. Parisi, L. Palatella, S. Pigolotti, A. Politi, A. Puglisi, L. Rondoni, S. Ruffo, M. Serva, A.Torcini, M. Vergassola and D. Vergni.

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