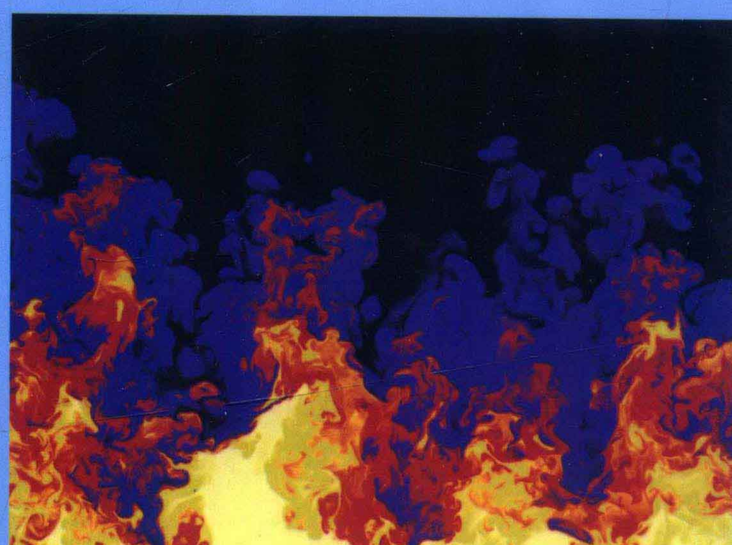
Luca Peliti

Statistical Mechanics in a Nutshell

简明统计力学



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Luca Peliti

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Statistical Mechanics in a Nutshell

Preface to the English Edition

Make things as simple as possible, but not simpler.
—*attributed* to Albert Einstein

The aim of the present book is to provide a concise introduction to statistical mechanics: a field of theoretical physics that has experienced tumultuous development in recent years. In the early 1970s, it was recognized that quantum field theory—the most widely accepted paradigm for the description of elementary particles—can be interpreted in a statistical mechanics language. This has allowed for extensive interchange of researchers and results between the two fields, leading to the impressive achievements of the modern theory of phase transitions. More recently, the intensive investigation of the statistical physics of disordered systems has led to the establishment of new methods and concepts, which have found surprising applications in a number of fields, ranging from economy (under the label of *econophysics*) to social sciences (*sociophysics*), to information processing. Meanwhile, within statistical physics proper, there has been a continuous interest in complex systems, especially of biological interest, and a new understanding of soft matter and of physical biology has arisen, thanks to newly developed theoretical tools and to the amazing advances in experimental techniques.

I am unable to provide a thorough introduction to these exciting developments in a short book kept at an elementary level. What I hope I have succeeded in doing is to introduce the reader to the basic concepts, to the essentials of the more recent developments, leaving her or him on the threshold of the different fields in which current research is most active. In view of this goal, the book is organized so that the first five chapters, which should be read sequentially, deal with the basic concepts and techniques of modern statistical mechanics, while the last five chapters, which can be read independently, each deal at an introductory level with a different aspect of interest in current research. I strived to keep the discussion at the most elementary level the subject could afford, keeping in mind the quotation in the epigraph.

"Every book is a collaborative effort, even if there is only one author on the title page" (M. Srednicki) [Sred06]. This book is no exception. A number of friends and colleagues have helped me collect my notes for their publication in the Italian edition of this book:

Stanislas Leibler, whose lecture notes were an important source of inspiration; Mauro Sellitto and Mario Nicodemi, who helped me with the first draft; and Antonio Coniglio, Franco Di Liberto, Rodolfo Figari, Jean-Baptiste Fournier, Silvio Franz, Giancarlo Franzese, Giuseppe Gaeta, Marc Mézard, Fulvio Peruggi, and Mohammed Saber, who provided a number of important suggestions and corrections. Further observations and comments on the published book were made to me by Jeferson Arenzon, Alberto Imparato, Andrea Longobardo, and a number of students of my courses. I am also grateful to Alberto Clarizia, Giancarlo D'Ambrosio, Pietro Santorelli, Maurizio Serva, and Angelo Vulpiani for discussions that have led me to reconsider some points of my exposition. Giuseppe Trautteur encouraged me to publish my lecture notes in book form and connected me with Alfredo Salsano at Bollati Boringhieri. I am grateful to Tony Zee for suggesting to publish the book in English and putting me in contact with Princeton University Press. A reader at the Press suggested adding the discussion of a few relevant points, which I did with great pleasure. I received from Natalie Baan, Ingrid Gnerlich, and Jennifer Harris all the help I could dream of during the production process. Mark Epstein was brilliantly able, not without effort, to transform my involved Italian into fluid English prose. Sarah Stengle designed the attractive jacket, based on an illustration of turbulent flow that was kindly provided by Guido Boffetta.

I renew the dedication of this book to Giovanni Paladin. We are still reaping the fruit of his scientific activity, so untimely and tragically interrupted.

Preface

I learned more from my pupils than from all others.
—Lorenzo Da Ponte

This work is a result of the notes I have gathered while preparing lessons in statistical mechanics—a course I have been teaching for 15 years at the Federico II University in Naples (Italy). The course's aim is to be both a beginner's and an advanced course. The first section therefore contains an introduction to the problems and methods of statistical mechanics, devised for students without any prior knowledge of the subject, while the second section contains an introduction to some topics of current interest. The work is structured accordingly, with a first group of chapters (1 to 5) that are meant to be studied sequentially, corresponding to the first section, while the following chapters can also be studied independently of one another.

This arrangement has led to a drastic shift in the presentation of the subject matter as compared to more traditional manuals. I thought it necessary to begin with a modern exposition of thermodynamics, using the geometric method introduced by J. W. Gibbs and reworked by L. Tisza and H. Callen. This work is therefore not merely another manual about thermodynamics, but an exposition that is quite innovative for texts at this level. It has significant conceptual and mnemonic advantages when compared to more traditional presentations. I have chosen to introduce the fundamental postulates of statistical mechanics on the basis of the expression of entropy in terms of the volume of the accessible phase space, due to Boltzmann. In this, I follow the point of view of L. D. Landau and S.-K. Ma. Although this point of view is not commonly represented in traditional texts, it allows one to do without the ergodic hypothesis, thus avoiding a series of delicate discussions that are ultimately not very relevant from a practical standpoint. In this manner, the basic techniques of statistical mechanics can be explained in their general outlines without taking too many detours. I have drastically simplified both the terminology and formalisms used in the definition of the fundamental ensembles, relying at every step on parallels with the formulation of thermodynamics I had previously introduced. I have experienced that this setting allows the teacher to reach in few lectures a point where the basic techniques can be used by the students to solve problems in elementary statistical mechanics (interaction-free systems). It is then possible to apply these techniques to simple physically interesting systems like quantum gases and paramagnets, and even to less traditional problems like the elasticity of polymers.

Working knowledge of methods for solving interaction-free systems is the foundation needed to introduce the most important method to explore the behavior of systems with interaction—in other words, *mean-field theory*. This theory is rarely mentioned in introductory statistical mechanics textbooks, and in my opinion, the space allocated to it in advanced textbooks is rarely sufficient. In my experience, it is not only fundamental, but it can be presented and understood at a beginner's level. It allows the teacher to introduce the problems connected to phase transitions and their fluctuations following a natural sequence; the phenomenological theory concerning these issues (*scaling*) is the final topic of the introductory section.

The second part of this work includes topics that can be studied independently from each other. The *renormalization group theory* of phase transitions represented a true conceptual revolution for our discipline. Explaining it is a notoriously difficult task, and I therefore attempt, in chapter 6, to present it in a manner that can be productive on a variety of levels. On the one hand, I explain its basic structure by introducing the concept of a Kadanoff transformation independent of its specific realizations, showing what the existence of this transformation entails for the system's critical behavior. I then introduce two of the transformation's concrete realizations: one elementary, but not systematic (decimation in the Ising model), and another that is more systematic—in the sense that it can lead to a series of successive approximations—even though it requires more complex calculations. In this case, it is important to transmit the method's principle, since its actual implementation is a more advanced topic, one that is also discussed in several other texts.

I devote one chapter to the modern theory of classical fluids, which has seen remarkable progress in the 1970s and 1980s. I believe that I have found a simple way to present the principles of diagrammatic development of the fluids' properties, as well as the derivation of integral equations. This is a good starting point to introduce more advanced methods, such as the density functional method.

Given the importance of numerical simulations in modern statistical mechanics, I devoted a chapter to this topic: I spend more time on basic problems than on the actual writing of simulation programs. This is a deliberate choice because discussing these programs would require the explicit introduction of a specific programming language, the analysis of a certain number of technical aspects related to its implementation, and so on—all items that would require too much space and distract the reader. Most often the students have already met some of these topics in other courses, and if this is not the case, discussing them would transform this chapter into a necessarily unsatisfactory introduction to the use of computers. On the other hand, I believe that discussions of the foundations of the Monte Carlo method, of the treatment of statistical errors, and above all of the extrapolation of the thermodynamic limit are of great relevance in the context of our discipline but are usually neglected in the textbooks of this level I have been able to examine. I have also insisted on the contribution that numerical simulation provides in clearing up problems in the foundations of statistical mechanics—a topic that as far as I know has been treated only in the text by S.-K. Ma [Ma85].

Another chapter is devoted to dynamic equilibrium phenomena, especially the theory of linear response and the fluctuation–dissipation theorem (and its consequences, such as the Onsager reciprocity relations). These topics are usually not treated in introductory textbooks at this level. My experience teaching the course has shown me that, starting with the theory of Brownian motion and making use of the concept of generalized Brownian motion, one can rapidly and easily derive these fundamental properties. Last, chapter 10 contains an introduction to the study of complex systems in statistical mechanics: it discusses the theory of linear polymers and then the theory of percolation as an example of a system with frozen disorder. It then contains a short introduction to the more general theory of disordered systems and allows a glimpse into one of its interdisciplinary applications—namely, the statistical theory of associative memories. In this fashion, the student can perceive the general nature of the methods of statistical mechanics, which the more traditional mechanistic approach instead tends to obscure.

In order to keep the size of the work within reasonable boundaries, I decided to omit the discussion of several interesting topics that are normally discussed in other similar textbooks. More specifically, I include only a brief introduction to the kinetic theory of gases (and I do not even mention Boltzmann's equation), I do not discuss the so-called ergodic problem, and I generally avoid discussions about the foundations of statistical mechanics. Indeed, the debate about these foundations is still ongoing but appears to me to bear little relevance for the concrete results that can be obtained within a more pragmatic approach. I also had to omit any reference to quantum statistical mechanics, except for those few cases that lead to calculations that are basically classical in nature. The problem is that, except for some special circumstances, this subject cannot be treated with the elementary methods I use in this textbook. This allows me to discuss the problems that lie at the heart of contemporary statistical mechanics, especially the theory of phase transitions and of disordered systems, with relative ease.

This book could not have been written without the help of many who helped and encouraged me in the course of these years. I especially thank Mauro Sellitto and Mario Nicodemi, who valiantly contributed to the completion of a first draft, as well as Stanislas Leibler, whose lessons inspired me when I was giving my course its shape. Many students in my statistical mechanics course contributed both to making certain proofs clearer and to reducing the number of errors. Although I cannot thank them all here one by one, I want to express my gratitude to all of them. I also thank Antonio Coniglio, Franco Di Liberto, Rodolfo Figari, Jean-Baptiste Fournier, Silvio Franz, Giancarlo Franzese, Giuseppe Gaeta, Marc Mézard, Fulvio Peruggi, and Mohammed Saber for their observations and suggestions, as well as Giuseppe Trautteur for his constant encouragement and for having suggested I publish my notes in book format.

I am grateful to the Naples Unit of the Istituto Nazionale di Fisica della Materia for the continuous aid they provided for my research during these years. I also thank the Naples Section of the Istituto Nazionale di Fisica Nucleare for the support they have provided.

This book is dedicated to the memory of Giovanni Paladin, whose curious and sharp mind promised great achievements for statistical mechanics, but one that a tragic fate has prematurely taken from us.

Statistical Mechanics in a Nutshell

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1 Introduction

Lies, damned lies, and statistics.

—Disraeli

1.1 The Subject Matter of Statistical Mechanics

The goal of statistical mechanics is to predict the macroscopic properties of bodies, most especially their thermodynamic properties, on the basis of their microscopic structure.

The macroscopic properties of greatest interest to statistical mechanics are those relating to *thermodynamic equilibrium*. As a consequence, the concept of *thermodynamic equilibrium* occupies a central position in the field. It is for this reason that we will first review some elements of thermodynamics, which will allow us to make the study of statistical mechanics clearer once we begin it. The examination of *nonequilibrium* states in statistical mechanics is a fairly recent development (except in the case of gases) and is currently the focus of intense research. We will omit it in this course, even though we will deal with properties that are time-dependent (but always related to thermodynamic equilibrium) in the chapter on dynamics.

The microscopic structure of systems examined by statistical mechanics can be described by means of mechanical models: for example, gases can be represented as systems of particles that interact by means of a phenomenologically determined potential. Other examples of mechanical models are those that represent polymers as a chain of interconnected particles, or the classical model of crystalline systems, in which particles are arranged in space according to a regular pattern, and oscillate around the minimum of the potential energy due to their mutual interaction. The models to be examined can be, and recently increasingly are, more abstract, however, and exhibit only a faint resemblance to the basic mechanical description (more specifically, to the quantum nature of matter). The explanation of the success of such abstract models is itself the topic of one of the more interesting chapters of statistical mechanics: the *theory of universality* and its foundation in the renormalization group.

The models of systems dealt with by statistical mechanics have some common characteristics. We are in any case dealing with systems with a large number of degrees of