Chapter 1

Introduction

When I was invited to consider writing a new book on non-equilibrium statistical mechanics, it did not take me much time to reach a positive decision. Several factors encouraged me to accept this challenge.

1) During my whole scientific life I have been deeply fascinated by the various aspects of our understanding of the macroscopic phenomena in terms of the behaviour of the underlying atoms or molecules. The *equilibrium properties* of matter (i.e., of a collection of N "atoms" enclosed in a region of volume V, where $N \gg 1$ and the volume is much larger than the volume of an atom) were already clearly formulated by *Gibbs* (1902) at the beginning of this century. The remarkable beauty of equilibrium statistical mechanics lies in the fact that *a single formula allows the calculation of all thermodynamical quantities from the input of the Hamiltonian, which defines in a nutshell the dynamics of the molecules.* If we ask, however, *how* the thermal equilibrium is reached (*if* it is reached at all) from an arbitrary starting point, this extraordinary simplicity no longer exists. A much more detailed study of the dynamics is now necessary, and this leads to an enormously more complex situation. It is precisely this feature which makes non-equilibrium statistical mechanics still a challenging field.

2) In 1963 I wrote a book on *Statistical Mechanics of Charged Particles* in which an early version of the new formalism (at that time) developed in Brussels for the non-equilibrium theory found a non-trivial application to plasmas. The latter systems offer an enormous amount of problems of highest interest, both for their theoretical and their practical importance.

3) In 1975 I published a rather voluminous treaty of *Equilibrium and Non-equilibrium Statistical Mechanics.* In this book, the main problems of the field were extensively treated. The non-equilibrium part of the book (almost one half) was developed in great detail, with an exposition of the derivation and the use of the "classical" kinetic equations for dilute gases, weakly coupled systems and plasmas. The matter was presented up to the end stage, i.e., the calculation of transport coefficients. This is the

final goal of non-equilibrium (kinetic) theory, which can be compared to experiment. Besides, the more "fundamental", hence more formal aspects of the theory have been treated rather extensively. I gave there a version of a general theory, to which I still adhere today (see Chap. 16).

4) In 1988 I wrote a book on *Transport Processes in Plasmas.* In its two volumes I covered only very partially this vast subject. Here, the emphasis was on a treatment leading from the appropriate kinetic equations (microscopic level) to explicit expressions of the transport coefficients.

5) Since more than 25 years I have been teaching statistical mechanics to Physics students at the Université Libre de Bruxelles.

Given these antecedents, it seemed rather easy to write a text on *Non-equilibrium* statistical mechanics, enclosed in a volume of about 300 pages. The book addresses persons who are familiar with the more elementary parts of equilibrium statistical mechanics: this is not, however, an indispensable requirement. The presentation given here is self-contained and should be understandable to any advanced undergraduate physics or engineering student having studied a course on Hamiltonian classical mechanics and of hydrodynamics.

The style is deliberately rather pragmatic. In other words, this book is not written for the "mathematically-minded" reader: the latter will find in the bibliographical notes citations of the works of that kind. The emphasis is put here on the physical aspects of the theory. The mathematical treatment is as clean as possible, without going into the full detail of ε-estimates, existence proofs, convergence proofs, etc. I do not question the importance of those aspects; but, besides my not being an expert in these matters, I believe that they tend to obscure the physics. Moreover, they are also limited to the very few highly idealized models that can be fully treated analytically.

My first approach was thus to try an expansion of my lecture notes, together with an update of the non-equilibrium part of my 1975 book, leaving aside the more formal aspects. It soon appeared, however, that a sufficiently complete coverage of the basic techniques together with a discussion of the most interesting applications (especially those developed in the last twenty years) led me very rapidly to a much longer text! If the exposition should retain a sufficient degree of detail in order to make it really self-contained, hence useful for the reader, a very drastic and painful selection had to be made among the matters treated.

After a long reflection, my decision was to *leave aside the quantum mechanical aspects* of the theory, and concentrate on CLASSICAL NON-EQUILIBRIUM STATISTICAL MECHANICS. The reasons motivating this choice can be summarized as follows.

A) Obviously, this decision left enough room for the treatment of a number of matters of great interest, which are presently at the forefront of research. These include topics such as transport in disordered systems, or in turbulent media, or in a fractal environment, transport and percolation, transport in chaotic systems, etc. *These problems do not appear to be treated in any presently existing general textbook of statistical mechanics.* On the other hand, these complex situations cannot be treated on a rigorous fundamental basis like the problems of "traditional" statistical mechanics: they require a more direct appeal to probabilistic concepts. In order to stress the inclusion of these "non-standard" subjects, I propose the unusual title "STATISTICAL DYNAMICS" for this book.

B) Quantum mechanics is not really necessary *per se* for understanding the fundamental nature of the irreversible behaviour of many-body systems: a classical description encompasses the main problems. This does not mean, of course, that quantum mechanics is unimportant: it is indispensable for the treatment of transport properties of high- and low-T_c superconductors, superfluids, spin glasses, etc. Thus, many important problems had to be, regretfully, left out of this book. The interested reader will find their treatment in textbooks on (what is now called) *materials science*, or *condensed matter physics.*

C) A good understanding of the methods of classical statistical mechanics allows an easy subsequent approach of the quantum formalism.

The book is structured as follows. It contains essentially three parts.

The *first part* covers Chaps. 2 - 4. Here the main tools of statistical mechanics are introduced. After a brief reminder of the dynamical laws governing the motion at the macroscopic level (hydrodynamical equations) and at the microscopic level (Hamiltonian dynamics), the description of matter in classical statistical mechanics is introduced in Chap. 3. The state of a many-body system must be represented by a new concept: the phase space distribution function. This allows us to ask new questions, making a smooth transition to macroscopic physics. The equation of evolution of this objec, i.e.,: the Liouville equation is, however, strictly equivalent to Hamiltonian dynamics. We also very briefly recall the main features of equilibrium theory.

The phase space distribution function is a very complicated object, depending on 10^{23} variables; its mathematical manipulation is heavy and delicate. Therefore, a much more convenient tool for the description of the state of large systems in terms of simple functions, that remain well-defined even in the thermodynamic limit of very large size and very large number of particles, is introduced in Chap. 4. The reduced distribution functions and the correlation functions will be used throughout the remainder of this book.

The *second part* covers Chaps. 5 - 10. Three classes of systems are considered here: they are sufficiently "simple" in order to allow a detailed and completely explicit mathematical treatment. In each of these, a small parameter can be defined and used for a kind of perturbative theory (to dominant order): the coupling parameter (weakly coupled systems), the density (dilute gases), and the plasma parameter (charged particles). Although it might appear that we introduced here a pedagogical simplification, the following point should be stressed. Besides three or four additional systems (mentioned briefly in the text), these are *the only systems for which an explicit kinetic equation is known.* Weakly coupled systems lead first to the mean field approximation (Chap. 5): although this is not yet a true kinetic equation, it yields the very important *Vlasov equation* of evolution. True kinetic equations include the effect of collisions: they are derived in Chap. 6 (*Landau equation* for a weakly coupled system), Chap. 7 (*Boltzmann equation* for a dilute gas), Chap. 8 (*Balescu-Lenard equation* for plasmas). Their common general properties, including their relation to irreversibility, dissipation and stochastic processes, are discussed in Chap. 9. Finally, Chap. 10 describes the transition to macroscopic hydrodynamics and *transport theory.* It illustrates the use of kinetic equations for concrete calculations of transport coefficients. All these treatments are in the line of "traditional" nonequilibrium statistical mechanics, in which one attempts to reach the ambitious goal of deriving macroscopic laws from molecular dynamics as "exactly" as possible. When trying to attack more complicated problems, it becomes impossible to adhere strictly to this discipline: one is bound to make some concessions. These consist of introducing from the outside some form of *a priori randomness.*

The *third part* of the book deals with these matters. Some of them are very old and classical; but they led to recent highly fascinating and non-trivial extensions. Chap. 11 treats the relation between transport and the stochastic description of the motion in terms of the *Langevin equation* or the associated *hybrid kinetic equation.* This subject has found a dynamical justification in the so-called Green-Kubo formulae for the transport coefficients. Chap. 12 deals with *Random Walks*; the stress is laid on the recent developments of the *Continuous Time Random Walks* and their relation to transport. This chapter introduces such non-standard topics as *"strange diffusion"* and shows the importance of non-markovian processes. Chaps. 13 and 14 deal with *critical phenomena*, as illustrated by their simplest appearance in the problem of *percolation.* The transport aspect of this problem introduces the problem of strange diffusion on fractal structures. Finally, a different type of simplification is used in Chap. 15: a complex dynamical system (but related to some concrete problems, like the behaviour of charged particles in a toroidal magnetic field configuration) is simplified to a *discrete low-dimensional map.* The well-known standard map offers some fascinating aspects related to transport: emergence of a truly diffusive regime in the limit of large stochasticity, but also strange diffusion in a regime of incomplete chaos.

In the concluding chapter, a brief discussion is given of several recent attempts toward a *general theory of irreversibility.* As stated above, the general outlook adopted in the present book is deliberately pragmatic; this discussion is therefore reduced to a minimum.

1.1 Bibliographical Notes BN1

The historical book of Gibbs is:

Gibbs, J.W., 1902, *Elementary Principles in Statistical Mechanics*, Yale Univ. Press, Yale, N.H., (reprinted by Dover, New York, 1960).

My previous books mentioned in the text are listed here, together with an appropriate abbreviation:

R. Balescu, 1963, *Statistical Mechanics of Charged Particles*, Interscience, New York, **(RB-1),**

R. Balescu, 1975, *Equilibrium and Nonequilibrium Statistical Mechanics*, Wiley-Interscience, New York, **(RB-2);** reprint: 1991, Krieger, Melbourne, Florida,

R. Balescu, 1988, *Transport Processes in Plasmas*, 2 volumes, (vol.1: *Classical Transport Theory,* vol. 2: *Neoclassical Transport Theory*), North Holland, Amsterdam, **(RB-3).**