Preface

The field of research presented in this book is born from a blending of ideas and techniques from statistical physics, dynamical systems theory, stochastic processes and computational physics. This combination suitably amends traditional statistical mechanics, which is a remarkably expedient tool for coping effectively with the presence of many degrees of freedom by applying probabilistic concepts. For a long time statistical mechanics focussed on a rather restricted class of systems in relatively simple situations such as fluids and crystalline solids at or near equilibrium. Today it is realized that systems involving only a few variables also exhibit *complex behavior* in the form of bifurcations, chaotic dynamics and fractal geometry characterized by sensitive dependence on initial conditions and parameters, and by random-looking evolution in time and space reminiscent of many-body systems. Such systems can be viewed as a "laboratory" in which questions that for a long time remained unsolved in statistical mechanics, such as the origin of irreversible entropy production and linear response, can be raised on a new basis and brought to their solution.

Since chaos appears to be ubiquitous at the level of the microscopic dynamics of single particles it should determine to a large extent macroscopic-level behavior, from the shape of probability distributions and values of transport coefficients in simple models to diffusion in nanopores, transport on vibratory conveyors and the active Brownian motion of biological entities. That way, the very origin of *irreversibility and transport* can be intimately related to the intrinsic complexity due to nonlinear interactions between the individual constituents forming a macroscopic system. This poses the challenge to modern statistical mechanics of explaining the macroscopic properties of matter starting from *microscopic deterministic chaos* in the equations of motion of many-particle systems.

This book highlights two very recent approaches towards a microscopic theory of macroscopic transport: One focuses on Hamiltonian dynamical systems under nonequilibrium boundary conditions, the other proposes a non-Hamiltonian approach to nonequilibrium situations created by, for example, electric fields and temperature or velocity gradients.

A surprising result related to the former approach is that, in low-dimensional periodic structures, transport coefficients can be fractal functions of control parameters. These *fractal transport coefficients* are the first central theme of our book. We exemplify this phenomenon by deterministic diffusion in a chaotic map, which generalizes the well-known problem of a random walk on the line by inclusion of memory effects. We then outline an arsenal of analytical and numerical methods for computing deterministic transport coefficients such as electrical conductivities and chemical reaction rates. These methods are applied to a hierarchy of nonlinear dynamical systems which successively become more complex, starting from abstract one-dimensional maps up to particle billiards that are directly accessible to experiments. In all cases the resulting transport coefficients turn out to be either fractal or to be at least profoundly irregular. We furthermore provide physical explanations for these fractalities.

The second central theme is a critical assessment of a non-Hamiltonian approach to nonequilibrium transport. Here we deal with situations where nonequilibrium constraints pump energy into a system, hence there must be some thermal reservoir that prevents a system from heating up. Very practical modelings of thermal reservoirs, which are widely used in molecular dynamics computer simulations, are Gaussian and Nosé-Hoover thermostats. Surprisingly, these approaches yield simple relations between fundamental quantities of nonequilibrium statistical mechanics and dynamical systems theory. This is due to the fact that these *thermostats* are *deterministic and time-reversible*, thus carrying over respective properties of Newton's equations of motion to nonequilibrium situations. This is in contrast to stochastic thermostats, which are recovered from them in case of memory loss at subsystem–reservoir couplings. Our goal is to critically assesses the universality of these results. As a vehicle of demonstration we employ the driven periodic Lorentz gas, a toy model for the classical dynamics of an electron in a metal under application of an electric field. Applying different types of thermal reservoirs to this system, we compare the resulting nonequilibrium steady states with each other. Along the same lines we discuss an interacting many-particle system under shear and heat. We then describe an unexpected relationship between deterministic thermostats and active Brownian particles modeling the motility of biological entities.

Related to these two main themes the book features a third part in which we outline very recent developments in this field. There is thus a chapter with mini-reviews on fluctuation relations, Lyapunov modes, Fourier's law and pseudochaotic transport connecting this work directly with highly active research areas that we feel are particularly interesting.

We argue that the theory presented in this book is particularly useful for the description of a novel class of systems, which is right in-between high- and low-dimensional, interacting and non-interacting many-particle systems. Such intermediate statistical dynamics may display both ordinary thermodynamic behavior as well as nontrivial nonlinear properties. Crosslinks to experiments are discussed throughout the whole work. Most of these experiments are on systems defined on meso to nanoscales. We thus presume that the theory outlined here should have further applications in the currently emerging field of the nanosciences. Understanding the basic physical principles of this theory may indeed help to "design" systems exhibiting specifically desired non-trivial properties. This point will be worth future exploration which, however, goes beyond the scope of this work.

A detailed outline of the contents of this book is presented in the introductory Chapter 1. Section 1.3 contains a guideline of how to read this book, some remarks on the style in which it is written and advice on required background knowledge. With this recipe, we hope that our book will provide a useful introduction for newcomers to this field as well as a reference and source of inspiration for established researchers.

This book is a profoundly amended and updated version of the author's habilitation thesis [Kla04a] summarizing about ten years of research. Such work would not have been possible without inspiring and fruitful collaboration with a large number of colleagues.

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