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Microscopic Chaos, Fractals and Transport in Nonequilibrium Statistical Mechanics

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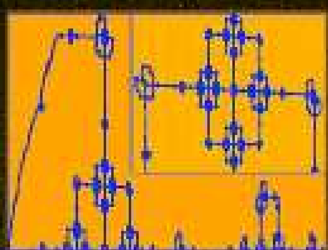

A valuable introduction for newcomers as well as an important reference and source of inspiration for established researchers, this book provides an up-to-date summary of central topics in the field of nonequilibrium statistical mechanics and dynamical systems theory.

Understanding macroscopic properties of matter starting from microscopic chaos in the equations of motion of single atoms or molecules is a key problem in nonequilibrium statistical mechanics. Of particular interest both for theory and applications are transport processes such as diffusion, reaction, conduction and viscosity.

Recent advances towards a deterministic theory of nonequilibrium statistical physics are summarized: Both Hamiltonian dynamical systems under nonequilibrium boundary conditions and non-Hamiltonian modelings of nonequilibrium steady states by using thermal reservoirs are considered. The surprising new results include transport coefficients that are fractal functions of control parameters, fundamental relations between transport coefficients and chaos quantities, and an understanding of nonequilibrium entropy production in terms of fractal measures and attractors.

The theory is particularly useful for the description of many-particle systems with properties in-between conventional thermodynamics and nonlinear science, as they are frequently encountered on nanoscales.

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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.

First of all, I would like to express my sincere appreciation and gratitude to Profs. S.Hess, J.R.Dorfman, T.Tél, P.Gaspard, and G.Nicolis, who allowed me to learn from them during my formation as a scientist. I owe them very much for their guidance. I furthermore wish to thank Prof. P.Fulde for supporting profoundly my research activities at the Max Planck Institute for the Physics of Complex Systems (MPIPKS) in Dresden.

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London, Winter 2006/2007 *Rainer Klages*

Chapter 1

*Introduction and outline

Statistical mechanics endeavours to understand the origin of macroscopic properties of matter starting from the microscopic equations of motion of single atoms or molecules. This program traces back to the founders of statistical mechanics, Boltzmann, Maxwell and Gibbs [Bol64; Max65a; Max65b; Gib60]. For many-particle systems in thermal equilibrium it was pursued with remarkable success [Tol38; Ehr59; Rei65; Hua87; Tod92]. However, in nonequilibrium situations, that is for systems under constraints such as external fields or by imposing temperature or velocity gradients, statistical mechanical theories appear to be rather incomplete: In contrast to the equilibrium case there is no generally accepted definition of a nonequilibrium entropy, and there is no general agreement on nonequilibrium ensembles that might replace the equilibrium ones [Pen79; Eva90b; Ger99; Rue99b; Gal99].

Fresh input concerning these fundamental problems came from the side of dynamical systems theory, in particular by works of mathematicians like Sinai, Ruelle, Bowen and others over the past decades [Sin91; Sin00; Rue78; Bow75]. Indeed, *SRB measures*[1] appear to be good candidates for taking over the role of the Gibbs ensemble in nonequilibrium [Gas98a; Dor99; Gal99; Rue99b; You02; Gal03b]. Additionally, the advent of powerful computers made it possible to numerically solve the nonlinear equations of motion of many-particle systems [All87; Eva90b; Hoo91; Hoo99]. This enabled to investigate the interplay between microscopic chaos in the collisions of single particles and transport properties on macroscopic scales in much more detail than it was possible to the times of the founders of statistical mechanics.

This book focuses on two basic approaches that evolved over the past

[1] The acronym stands for the initials of Sinai, Ruelle and Bowen.

two decades trying to develop a concise picture of nonequilibrium statistical mechanics by employing methods of dynamical systems theory. In the following two introductory sections we summarize important features of these two directions of research. We then sketch how this book is embedded into the existing literature, outline in more detail its contents and say some words about the style in which it is written. The hurried reader may wish to immediately pick up the *red thread through this book* provided in Section 1.3.

1.1 Hamiltonian dynamical systems approach to nonequilibrium statistical mechanics

In recent work, Gaspard, Nicolis and Dorfman studied nonequilibrium situations by imposing specific boundary conditions onto spatially extended chaotic *Hamiltonian* (-like) dynamical systems. A typical example is diffusion processes due to concentration gradients at the boundaries. By this approach the macroscopic transport properties of deterministic dynamical systems could be linked to the underlying microscopic chaos in the equations of motion of the single particles in two ways: The *escape rate formalism* considers dynamical systems with absorbing boundaries [Gas90; Gas92c; Gas93; Gas95b; Dor95; Gas95c; Gas98a; Dor99]. Here the escape rate determined by a statistical physical transport equation such as, for example, the diffusion equation, is matched to the one calculated from the Liouville equation of the dynamical system. This procedure yields simple formulas linking transport coefficients to dynamical systems quantities, which are here the positive Lyapunov exponents and the Kolmogorov-Sinai entropy of the dynamical system or the fractal dimension of the repeller associated with the open system.

A second, conceptually related approach applies to closed systems with periodic boundary conditions. It has been worked out for diffusion [Gil01; Gas01] and for reaction-diffusion [Cla02] in low-dimensional models. In this case the decay rate to thermal equilibrium obtained from the reaction-diffusion equation is related to the fractal dimension of the corresponding *hydrodynamic mode* in the Liouville equation of the dynamical system. The transport coefficients can thus be expressed as functions of the system's largest Lyapunov exponent combined with the Hausdorff dimension of this mode. Both approaches can consistently be derived by using Ruelle's thermodynamic formalism [Gas95c; Gas01].

Along similar lines the origin of nonequilibrium entropy production in chaotic dynamical systems has been investigated. Here the analysis of transport in two-dimensional *multibaker maps*, introduced by Gaspard [Gas92a], played a crucial role. Multibakers are deterministic versions of random walks on the line, where stochasticity is replaced by microscopic chaos. On the other hand, these maps share generic properties with Hamiltonian particle billiards of which *Lorentz gases* [Lor05] are typical examples. In these models a moving point particle collides elastically with circular scatterers distributed randomly or periodically in space. The periodic version with applied external field is also known as the *Galton board* [Gal77]. Both multibakers and Lorentz gases became paradigmatic models in the field of chaos and transport [Gas98a; Dor99; Hoo99; Sza00; Kar00; Gar02; Vol02].

For nonequilibrium transport in such systems, Tél, Vollmer, Breymann and Mátyás [Bre96; Tél96; Vol97; Bre98; Vol98; Tél00; Vol00; Mát01; Vol02; Vol04; Mát04b] as well as Gaspard, Tasaki, Dorfman and Gilbert [Gas97b; Gil99a; Tas99; Tas00; Gil00a; Gil00b; Dor02] proposed new concepts for defining *coarse-grained Gibbs entropies* leading to a nonequilibrium entropy production that is in agreement with irreversible thermodynamics. The former group attributed the source of irreversible entropy production to the chaotic mixing of dynamical systems and to the associated loss of information due to coarse graining. The latter authors argued that the singularity of the SRB measures exhibited by these nonequilibrium systems already necessitates a respective coarse graining for mathematical reasons. In both approaches, the source of irreversible entropy production is thus identified with the fractal character of these SRB measures.

Cohen and Rondoni, on the other hand, criticized both theories starting from the fact that the simple models to which these analyses were applied consist of moving point particles that do not interact with each other but only with fixed scatterers [Coh98; Ron00a; Coh02; Ron02b]. In their view these systems are non-thermodynamic models, which do not allow to identify local thermodynamic equilibrium or any proper source of thermodynamic entropy production. These arguments have been critically analyzed in Refs. [Vol02; Dor02; Tél02; Gas02a; Gas03].

Another important topic associated with the Hamiltonian approach to nonequilibrium transport concerns the *parameter dependence of transport coefficients*. It originated from studying deterministic transport in simple one-dimensional chaotic maps periodically continued on the line [Sch89; Kla96b; Gas98a; Dor99; Cvi07]. Specific types of such models can straightforwardly be derived from the multibaker maps mentioned above [Gas92a; Gas98a; Dor99]. There exists quite an arsenal of methods to compute deterministic diffusion coefficients for these maps, such as transition matrix methods [Gas92a; Cla93; Kla95; Kla96b; Kla97; Gas98c; Gas98a; Kla99a; Koz99; Kla02a; Yos06; Bar05; Bar06], systematic evaluations starting from Taylor-Green-Kubo formulas [Kla96b; Dor99; Gas98c; Kla02d; Kor02; Kor04b], rigorous mathematical treatments related to kneading sequences [Gro02], cycle expansion methods [Art91; Art93; Art94; Tse94; Che95a; Gas98a; Cvi07; Cri06] and techniques employing the thermodynamic formalism [Sto94; Sto95a; Sto95c; Sto95b; Rad97]. Using such methods to calculate the parameter-dependent deterministic diffusion coefficient of a simple one-dimensional map, the result was found to be a fractal function [Kla03; Koz04; Kel07] of a control parameter [Kla95; Kla96b; Kla99a]. This forms the main theme of Chapter 2. The origin of this fractality can be traced back to the existence of long-range dynamical correlations in the microscopic dynamics of the moving particle [Kla96b; Kla02d]. These correlations are topologically unstable and change in a complicated way under parameter variation, a phenomenon that is known as “pruning” in periodic orbit theory [Cvi07].

Starting from this observation, both the electrical conductivity [Gro02] and the chemical reaction rate [Gas98c] of related maps were found to be fractal functions of control parameters, see Chapters 3 and 4. The drift-diffusion coefficient furthermore exhibits phase locking, and the nonlinear response turns out to be partly negative. The latter fact can be understood by relating the biased model to deterministic ratchets, see Section 3.4, for which the existence of current reversals under parameter variation is a characteristic property [Jun96; Hän96; Rei02].

Similar fractal transport properties were detected for phase diffusion in a time-discrete model of a driven nonlinear pendulum [Kor02; Kor04b], see Chapter 6. In this case bifurcation scenarios generate a complicated interplay between normal and anomalous diffusive dynamics. Analogous equations have been studied in the context of experiments on Josephson junctions [Jac81; Cir82; Mir85; Mar89; Wei00; Tan02d], on superionic conductors [Ful75; Bey76; Mar86] and on systems exhibiting charge-density waves [Bro84]. A related phenomenon has recently been discussed for a toy model of nanoporous material, which motivated the introduction of different notions of complexity [Jep06].

Purely anomalous dynamics is the subject of the second half of Chapter 6. There it is shown that an intermittent subdiffusive map exhibits fractal parameter dependencies of a suitably generalized diffusion coefficient [Kor05]. This establishes an interesting crosslink to the very active field of *anomalous transport* for which a rich arsenal of stochastic methods is available while approaches by dynamical systems theory are currently being developed [Gas88; Wan89b; Wan89a; Wan93; Sto95b; Art93; Art97a; Cvi07; Det97a; Det98; Art03; Art04; Tas02; Tas04].

In view of experimental situations one may ask to which extent fractal transport coefficients are robust with respect to imposing *random perturbations* in space and time onto the underlying models. This connects the present line of research to the fields of disordered [Rad96; Rad99; Rad04; Fic05], respectively noisy [Gei82; Rei94; Rei96a; Rei96b; Fra91; Wac99; Cvi00] dynamical systems. A first answer to this question is provided by Chapter 5 in that the oscillatory structure of the diffusion coefficient of a simple model gradually “smoothes out” by increasing the perturbation strength, eventually recovering precise agreement with results from stochastic theory [Kla02b; Kla02c].

In order to move fractal transport coefficients to more realistic physical systems, studies of *deterministic transport in Hamiltonian particle billiards* were put forward. In the periodic Lorentz gas long-range dynamical correlations have again a profound impact on the parameter dependence of the diffusion coefficient [Kla00a; Kla02d]. This effect was found to be even more pronounced in a billiard with scatterers of flower-shaped geometry [Har02] and in a periodically corrugated floor, where particles move under the action of a gravitational force [Har01]. This forms the contents of Chapters 7 and 8.

We remark that billiards of Lorentz gas-type can actually be manufactured and studied experimentally in form of semiconductor antidot lattices, where noninteracting electrons move quasi-classically under application of external electric and magnetic fields [Wei91; Lor91; Wei95; Wei97]. Indeed, the measured magnetoresistance of such systems is well-known to be a highly irregular function of the field strength. For specific settings this quantity has theoretically been predicted to be fractal [Wie01]. Similar periodic structures are present in meso-, micro and nanoporous crystalline solids, which have wide-ranging industrial applications, for example, as molecular sieves, adsorbants and catalysts [Kär92; Sch03a]. Techniques and results that are connected to the ones summarized in Chapter 7 are indeed available in literature on diffusion in zeolites, see Chapter 8 for details.

Another link between fractal transport coefficients and physical reality is provided by the bouncing ball billiard introduced in Chapter 9, which models *deterministic diffusion of granular particles* on a vibrating periodically corrugated floor. Simulations of this system revealed again highly irregular diffusion coefficients, which are here particularly due to phase locking and related resonances [Mát04a; Kla04b]. This model was constructed in order to be relevant to recent experiments on granular material diffusing on vibrating surfaces [Far99; Pre02]. It also describes the very practical problem of transport of granular particles on vibratory conveyor belts [Per92; Han01; Gro03; Gro04].

To finish this brief outline of a Hamiltonian dynamical systems approach to nonequilibrium statistical mechanics, as far as it relates to this book, we refer to an interesting experiment by Gaspard et al. [Gas98b; Bri01]. Its purpose was to verify the existence of microscopic deterministic chaos in the Brownian motion of an interacting many-particle system. Long trajectories of a tracer particle suspended in a fluid were recorded, and the data analysis yielded a non-zero sum of positive Lyapunov exponents. Hence the existence of an exponential dynamical instability underlying many-particle diffusion, that is, chaos in the sense of Lyapunov, was concluded. This finding motivated the study of diffusion in models without Lyapunov dynamical instabilities. These "nonchaotic" models yielded results that were indistinguishable from the experimental data and were thus presented as counterexamples [Det99b; Gra99; Det00b].

As we will show in Chapter 17, such models belong to an interesting class of systems exhibiting what one may call *pseudochaotic transport* [Zas03], where dynamical randomness is generated by mechanisms that are weaker than exponential dynamical instabilities. Other prominent examples are polygonal billiard channels [Alo02; Jep06; San06], for which both normal diffusion and normal heat conduction have been verified numerically [Li02; Li03a]. The latter studies point towards another broad field of research, which tries to learn about the necessary and sufficient conditions for the existence of *Fourier's law* [Bon00b; Lep03; Pro05]. Starting from harmonic and anharmonic chains up to thermal conduction in particle billiards like Lorentz and rotating disk channels, we will review some aspects of this research in the same chapter.

1.2 Thermostated dynamical systems approach to nonequilibrium statistical mechanics

A nontrivial limitation of the Hamiltonian approach to chaotic transport is that it excludes nonequilibrium constraints generating a continuous flux of energy into the system as, for example, the application of external fields.[2] Such situations necessitate the modeling of an infinite dimensional *thermal reservoir* , which is able to continuously absorb energy in order to prevent a subsystem from heating up [Pen79; Rue99b; Gal99; Dor99; Ron02a]. The need to model these situations emerged particularly from *nonequilibrium molecular dynamics computer simulations*, which focus on simulating heat or shear flow of many-particle systems or currents under application of external fields [Eva90b; Hoo91; Hes96a; Mor98; Hoo99; Det00a; Mun00; Tuc00].

A well-known example for a modeling of thermal reservoirs is provided by the *Langevin equation* [Lan08] yielding the interaction with a heat bath by a combination of Stokes friction and stochastic forces [Wax54; Rei65; Pat88; Kub92; Zwa01]. One way to derive generic types of Langevin equations starts from a Hamiltonian formulation for a heat bath consisting of infinitely many harmonic oscillators. This heat bath suitably interacts with a subsystem that consists of a single particle [Zwa73; For87; Kub92; Stu99; Zwa01]. In the course of the derivation the detailed bath dynamics is eliminated resulting in an equation of motion for the subsystem that is *non-Hamiltonian*. The Langevin equation thus nicely illustrates Ruelle's statement "if we want to study non-equilibrium processes we have thus to consider an infinite system or non-Hamiltonian forces" [Rue99a], see Chapter 10.[3]

As we will argue in the second part of this book, there is nothing

[2] Note that the use of *Helfand moments* enables an indirect treatment of such situations similar to the use of equilibrium time correlation functions related to Green-Kubo formulas [Dor95; Gas98a].

[3] For a related statement see, e.g., Smale [Sma80]: "We would conclude that theoretical physics and statistical mechanics should not be tied to Hamiltonian equations so absolutely as in the past. On physical grounds, it is certainly reasonable to expect physical systems to have (perhaps very small) non-Hamiltonian perturbations due to friction and driving effects from outside energy absorbtion. Today also mathematical grounds suggest that it is reasonable to develop a more non-Hamiltonian approach to some aspects of physics." Smale further suggests to "revive the ergodic hypothesis via introduction of a dissipative/forcing term" into Hamiltonian equations of motion, since in his view dissipative dynamical systems have a better chance to be ergodic than Hamiltonian ones, which usually exhibit profoundly non-ergodic dynamics due to a mixed phase space.

mysterious in modeling thermal reservoirs with non-Hamiltonian equations of motion, in line with Refs. [Pen79; Sma80; Che95b; Rue96; Gal99; Lie99; Ron02a]. In case of thermostated systems the non-Hamiltonianity straightforwardly results from projecting out spurious reservoir degrees of freedom. Early nonequilibrium molecular dynamics computer simulations employed stochastic models of heat baths [And80; Cic80; Sch78; Ten82; All87; Nos91], which were partly considered to be inefficient. Infinite-dimensional Hamiltonian thermal reservoirs, on the other hand, can very well be modeled and analyzed analytically [Eck99b; Eck99a; Zwa01], but on a computer the number of degrees of freedom must, for obvious reasons, remain finite. These constraints provided a very practical motivation for constructing nonequilibrium steady states on the basis of *finite-dimensional, deterministic, non-Hamiltonian equations of motion.*

About twenty-five years ago Hoover et al. [Hoo82] and Evans [Eva83a] came up with a strikingly simple non-Hamiltonian modeling of a thermal reservoir, which they coined the *Gaussian thermostat* [Eva83b]. This scheme introduces a (Gaussian) constraint in order to keep the temperature for a given subsystem strictly constant in nonequilibrium at any time step. A few years later Nosé invented a closely related non-Hamiltonian thermal reservoir, which was able to thermostat the velocity distribution of a given subsystem onto the canonical one in equilibrium and to keep the energy of a subsystem constant on average in nonequilibrium [Nos84a; Nos84b]. His formulation was simplified by Hoover [Hoo85] leading to the famous *Nosé-Hoover thermostat* [Eva90b; Hoo91; Hes96a; Mor98; Hoo99; Det00a; Mun00; Ron02a].

Suitable adaptations of these schemes to nonequilibrium situations such as, e.g., shear flows yielded results that were well in agreement with predictions of irreversible thermodynamics and linear response theory [Eva90b; Sar98]. Hence, these thermostats became widely accepted tools for performing nonequilibrium molecular dynamics computer simulations. Eventually, they were successfully applied even to more complex fluids such as, for example, polymer melts, liquid crystals and ferrofluids [Hes96a; Hes96b; Hes97], to proteins in water and to chemical processes in the condensed matter phase [Tuc00]. These two schemes are introduced and analyzed in detail in Chapters 11 and 12.

Soon it was realized that a non-Hamiltonian modeling of thermal reservoirs not only enabled the efficient construction of nonequilibrium steady states on the computer but also that it made them amenable to an analysis by dynamical systems theory [Eva90b; Hoo91; Mar92a;

Mar97; Tél98; Mor98; Hoo99]. First of all, in contrast to the stochastic Langevin equation Gaussian and Nosé-Hoover thermostats preserve the deterministic nature of the underlying Newtonian equations of motion. Furthermore, although the resulting dynamical systems are dissipative, surprisingly the thermostated equations of motion are still time-reversible hence yielding a class of systems characterized by the, at first view, contradictory properties of being *time-reversible, dissipative* and, under certain circumstances, even being *ergodic* [Che95b; Che97; Hoo96b]. Computer simulations furthermore revealed that subsystems thermostated that way contract onto *fractal attractors* [Hol87; Mor87a; Mor87b; Hoo87; Pos88; Mor89a; Pos89] with an *average rate of phase space contraction that is identical to the thermodynamic entropy production* [Hol87; Pos88; Che93a]. This led researchers to conclude that in thermostated dynamical systems the phase space contraction onto fractal attractors is at the origin of the second law of thermodynamics [Hol87; Rue96; Rue97c; Rue97b; Hoo99; Gal98; Gal99].

Interestingly, the average rate of phase space contraction plays the same role in linking statistical physical transport properties to dynamical systems quantities as the escape or decay rates in the Hamiltonian approach to nonequilibrium [Tél96; Rue96; Bre98; Gil01]. The key observation is that, on the one hand, the average phase space contraction rate is identical to the sum of Lyapunov exponents of a dynamical system, whereas, on the other hand, for Gaussian and Nosé-Hoover thermostats it equals the thermodynamic entropy production. For thermostated dynamical systems this again furnishes a relation between transport coefficients and dynamical systems quantities [Mor87a; Pos88; Eva90a; Van92]. A suitable reformulation of these equations makes them formally analogous to the ones obtained from the Hamiltonian approach to transport. These results were considered as an indication of the existence of a specific backbone of nonequilibrium transport in terms of dynamical systems theory [Tél96; Bre98; Gas98a; Gil01]. This discussion is summarized in Chapter 13.

Another interesting feature of Gaussian and Nosé-Hoover thermostated dynamical systems is the existence of *generalized Hamiltonian and Lagrangian formalisms* from which the thermostated equations of motion can be deduced, which involve non-canonical transformations of the phase space variables [Nos84a; Nos84b; Det96b; Det97b; Mor98; Cho98]. Similarly to Hamiltonian dynamics, deterministically thermostated systems often share a certain symmetry in the spectrum of their Lyapunov exponents known as the *conjugate pairing rule*, which was widely studied in the recent literature [Dre88; Pos88; Eva90a; Mor98; Sea98; Rue99b]. That is, all Lyapunov exponents of a given dynamical system can be grouped into pairs such that each pair sums up to the same value, which in nonequilibrium is non-zero.

In most cases Lyapunov exponents of thermostated systems can only be calculated numerically. For Lorentz gases and related systems, however, an analytical kinetic theory approach is available [vB95; Lat97; vB97; Del97b; vB98; Mül04]. Furthermore, in recent computer simulations of interacting many-particle systems Posch et al. [Mil98a; Pos00a; Mil02; Hoo02c; For04] observed the existence of *Lyapunov modes* in thermal equilibrium indicating that the microscopic contributions to the Lyapunov instability of a many-particle fluid form specific modes of instability, quite in analogy to the well-known hydrodynamic modes governing macroscopic transport [Eck00; McN01; Tan02c; Mar04; dW04a; Tan05a; Tan05b]. We will further elaborate on these findings in Chapter 17.

Such interesting properties inspired mathematicians to look at these systems from a rigorous point of view. A cornerstone is the proof by Chernov et al. of the existence of Ohm's law for the periodic Lorentz gas driven by an external electric field and connected to a Gaussian thermostat [Che95b; Che97]. Another important development was the *chaotic hypothesis* by Gallavotti and Cohen [Gal95a; Gal95b; Gal98; Gal99], which was motivated by results from computer simulations on thermostated dynamical systems [Eva93]. This fundamental assumption generalizes Boltzmann's ergodic hypothesis in summarizing some general expectations on the chaotic nature of interacting many-particle systems which, if fulfilled, considerably facilitate calculations of nonequilibrium properties; see the beginning of Chapter 18 for details and for what may represent a general picture of a chaotic dynamical systems approach to nonequilibrium statistical mechanics.

A rapidly developing field of research is that of nonequilibrium *fluctuation relations*, which establish simple symmetry relations between positive and negative fluctuations of nonequilibrium entropy production. A first version of such laws again came up within the framework of nonequilibrium molecular dynamics computer simulations for thermostated systems [Eva93; Eva94; Eva02b]. Later on different formulations of *fluctuation theorems* were proven on the basis of the chaotic hypothesis [Gal95a; Gal95b], for stochastic systems [Kur98; Leb99] and for Gibbs measures [Mae99]. Another type of fluctuation relations emerged at first quite independently from these theorems: The *Jarzynski work relation* connects equilibrium with nonequilibrium statistical mechanics by suggesting to extract equilibrium free energy differences from irreversible work performed in a nonequilibrium situation [Jar97b]. A link between this relation and fluctation theorems was later on realized in form of the *Crooks relation* [Cro99; Cro00].

Meanwhile fluctuation relations have been verified for many different systems in many different ways analytically and in computer simulations [Kur05; Eva02b; Ron02a; Jar02] as well as in experiments [Cil98; Wan02; Rit03; Bus05]. It appears that they belong to the rather few general results characterizing nonequilibrium steady states very far from equilibrium thus generalizing Green-Kubo formulas and Onsager reciprocity relations, which can be derived from them close to equilibrium. Chapter 17 provides a short introduction to this interesting new research topic.

1.3 The red thread through this book

The emphasis of this book is on two themes, which are intimately connected with the two directions of research outlined above: Part 1 elaborates on the calculation and explanation of fractal transport coefficients in low-dimensional deterministic dynamical systems. Part 2 deals with the construction and analysis of nonequilibrium steady states in dissipative dynamical systems associated with thermal reservoirs. On the basis of these discussions, Part 3 provides an outlook towards further important directions of research within the field of chaos and transport, summarizes all results and concludes with a number of open questions.

For a quick reading one is recommended all parts marked with a star (*), supplemented by studying the introductory remarks preceding all the single chapters. Sections labeled by a plus (+) contain advanced material that may be left for thorough studies. We highly recommend inclusion of the full Chapter 2 in such a quick reading. This chapter summarizes the major finding of the author's Ph.D. thesis work, which is the existence of a fractal diffusion coefficient in a very simple deterministic map. This map is a paradigmatic model motivating many of the investigations reported in Part 1. It furthermore exemplifies a deterministic approach towards nonequilibrium transport. The central aim of the work compiled in Chapters 3 to 9 is to bring fractal diffusion coefficients to physical reality. This requires a sharpening of the theoretical methods, which goes hand in hand with studying a series of increasingly more complex models. In the course of these efforts, analogous fractal properties were discovered for additional deterministic transport coefficients and in more complicated settings. Our main conclusion is that fractal transport coefficients are typical for a specific class of physical dynamical systems, and that they should be seen in experiments. To systematically argue for this statement is the main task of Part 1.

Concerning Part 2, we suggest that one goes at least through Section 10.1, which motivates the physics of thermal reservoirs in an intuitive way. The patient reader may wish to consult as well Section 10.2 for a more detailed motivation, which starts from the well-known Langevin equation by pointing towards some fundamental problems in modeling thermal reservoirs. If yet more time is left, we recommend taking a look at Chapter 11, which describes a paradigmatic modeling of a deterministic and time-reversible thermal reservoir. Applying this method to a simple model in a nonequilibrium situation, we summarize the resulting chaos and transport properties of the combined system in this chapter. Some researchers have argued that these properties should be universal for thermostated dynamical systems in nonequilibrium steady states altogether, see Chapters 11 to 13. Hence, the main theme of Part 2 is to critically assess the universality of these results as obtained from a non-Hamiltonian approach to nonequilibrium steady states. In Chapters 14 to 15 we show that there exist thermal reservoirs yielding counterexamples to most of these claims of universality. Chapter 16 then establishes a previously unexpected relationship between deterministic thermal reservoirs and simple models for the motility of biological entities such as, e.g., migrating cells.

The first chapter of the final Part 3 contains a very brief non-technical outline of four different research topics, which emerged particularly over the past few years. We emphasize that the corresponding single sections are not designed to provide in-depth reviews of these very active research areas. However, they might be of interest for researchers who are willing to take a bird's-eye view on what we consider to be very stimulating new developments in this field. These introductions might also be suitable for graduate students who want to enter these topics, e.g., in order to prepare for seminar talks or as a starting point for some research project. All four sections can be read independently.

As far as the style of this book is concerned we remark that all three parts are of a somewhat different nature. In a way, there exists a gradient of technicality, which is reflected in the degree of difficulty the non-expert may expect by reading through this book: Part 1 is the most technical one. Here the reader may enjoy learning about deterministic transport along the lines of hermeneutics: That is, the main models, methods and findings are presented from successively different points of views thus providing themes and variations that the reader will hopefully find interesting. Part 2 is written in a more pedagocial way. Here we try to keep things as simple as possible and do not present more technical details than absolutely necessary. Consequently there are only few formulas in this part but many figures and a lot of text. Part 3 is even less technical than Part 2. We remark that the first two parts contain a number of previously unpublished results, see particularly Chapter 3 and Sections 14.1 as well as 16.3.

All three parts presuppose some basic knowledge of (nonequilibrium) statistical mechanics [Rei65; Hua87] and of dynamical systems theory [Sch89; Eck85; Ott93; Bec93; All97; Tél06]. We touch upon some rigorous mathematics particularly in Section 3.2.1, otherwise our work represents a generic theoretical physicist's approach towards chaos and transport in nonequilibrium statistical mechanics, which does not require a detailed knowledge of mathematical dynamical system's theory. In this respect, we remark that for Part 2 we do not explicitly develop concepts such as SRB measures and Anosov systems, despite the fact that all issues discussed in this part are intimately related to them. We emphasize that these objects do play a crucial role for building up a more mathematical theory of nonequilibrium steady states [Gas98a; Dor99; Gal99; Rue99b]. However, in Part 2 we work on a level that is more applied consisting of straightforward physical examples and demonstrations combined with simple calculations and results from computer simulations. It is our hope that this approach still suffices to make the reader familiar with what we believe are some central problems in the field of chaos and transport in thermostated dynamical systems.

Books and reviews that are closely related to the topics covered by this work are particularly Refs. [Kla96b; Gas98a; Nic98; Dor99; Cvi07] for Part 1 and Refs. [Eva90b; Hes96a; Mor98; Hoo99; Det00a; Ron02a] for Part 2. There also exists a number of conference proceedings and related collections of articles, which the reader may wish to consult [Mar92a; Mar97; Tél98; Kar00; Sza00; Gar02; Kla04c]. We tried to be quite exhaustive as far as literature is concerned that we feel is especially relevant to the problems highlighted in this book, which resulted in the compilation of more than 800 references. However, it is impossible to be complete, and we apologize in advance for any important work that may have escaped our attention. We hope that this long bibliography will serve as a useful source of information for scientists doing research in this field. We also remark that in this book we usually do not intend to give historical accounts of developments in chaos theory and nonequilibrium statistical mechanics; for this purpose see, e.g., Refs. [Bru76; Gle88; Cvi07; Uff01]. Only on rare occasions do we go a little bit more into historical depth. Finally, there is a website available for this book, which will be kept up to date concerning comments, amendments or possible corrections, please see www.maths.qmul.ac.uk/∼klages/cftbook for further information.