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This book describes recent advances in the application of chaos theory to classical scattering and nonequilibrium statistical mechanics generally, and to transport by deterministic diffusion in particular.

The author presents the basic tools of dynamical systems theory, such as dynamical instability, topological analysis, periodic-orbit methods, Liouvillian dynamics, dynamical randomness and large-deviation formalism. These tools are applied to chaotic scattering and to transport in systems near equilibrium and maintained out of equilibrium. Chaotic scattering is illustrated with disk scatterers and with examples of unimolecular chemical reactions and then generalized to transport in spatially extented systems. Transport and chaotic properties are inter-connected. The phenomenological laws of hydrodynamics and of irreversible thermodynamics are derived from first principles defined in dynamical systems theory. The foundations of statistical mechanics are discussed on the basis of the hypothesis of microscopic chaos.

This book will be of interest to researchers interested in chaos, dynamical systems, chaotic scattering and statistical mechanics in theoretical, computational and mathematical physics and also in theoretical chemistry.

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More information

Contents

Preface *xvii*
Introduction *1*

Chapter 1 **Dynamical systems and their linear stability** *12*

1.1 Dynamics in phase space *12*
1.1.1 *The group of time evolutions* *12*
1.1.2 *The Poincaré map* *13*
1.1.3 *Hamiltonian systems* *14*
1.1.4 *Billiards* *15*
1.2 Linear stability and the tangent space *15*
1.2.1 *The fundamental matrix* *15*
1.2.2 *Lyapunov exponents* *16*
1.2.3 *Decomposition of the tangent space into orthogonal directions* *17*
1.2.4 *Homological decomposition of the multiplicative cocycle* *19*
1.2.5 *The local stretching rates* *20*
1.2.6 *Stable and unstable manifolds* *22*
1.3 Linear stability of Hamiltonian systems *23*
1.3.1 *Symplectic dynamics and the pairing rule of the Lyapunov exponents* *23*
1.3.2 *Vanishing Lyapunov exponents and the Lie group of continuous symmetries* *23*
1.3.3 *Hamilton–Jacobi equation and the curvature of the wavefront* *25*

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Pierre Gaspard
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1.3.4 *Elimination of the neutral directions* 28
1.3.5 *The local stretching rate in $f = 2$ hyperbolic Hamiltonian systems* 29
1.4 Linear stability in billiards 31
1.4.1 *Some definitions* 32
1.4.2 *The second fundamental form* 33
1.4.3 *The tangent space of the billiard* 33
1.4.4 *Free flight* 34
1.4.5 *Collision* 35
1.4.6 *Expanding and contracting horospheres* 36
1.4.7 *Two-dimensional hard-disk billiards ($f = 2$)* 39

Chapter 2 **Topological chaos** 43

2.1 Topology of trajectories in phase space 43
2.1.1 *Phase portrait and invariant set* 43
2.1.2 *Critical orbits: stationary points and periodic orbits* 44
2.1.3 *Nonwandering sets* 44
2.1.4 *Locally maximal invariant sets and global stability* 45
2.1.5 *Dense orbits and transitivity* 46
2.1.6 *Attractors, anti-attractors, and repellers* 46
2.2 Hyperbolicity 47
2.2.1 *Definition* 47
2.2.2 *Escape-time functions* 49
2.2.3 *Anosov and Axiom-A systems* 50
2.3 Markov partition and symbolic dynamics in hyperbolic systems 52
2.3.1 *Partitioning phase space with stable and unstable manifolds* 52
2.3.2 *Symbolic dynamics and shift* 53
2.3.3 *Markov topological shift* 55
2.4 Topological entropy 57
2.4.1 *Nets and separated subsets* 58
2.4.2 *Definition and properties* 58
2.5 The spectrum of periodic orbits 60
2.5.1 *Periodic orbits and the topological zeta function* 60
2.5.2 *Prime periodic orbits and fixed points* 61
2.5.3 *How to order a sum over periodic orbits?* 63
2.5.4 *The topological entropy of a hyperbolic invariant set* 64
2.6 The topological zeta function of hyperbolic systems 64

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0521018250 - Chaos, Scattering and Statistical Mechanics
Pierre Gaspard
Frontmatter
More information

2.6.1 *The topological zeta function for a nonoverlapping partition* 65
2.6.2 *The topological zeta function for an overlapping partition* 65

Chapter 3 **Liouvillian dynamics** 67

3.1 Statistical ensembles 67
3.2 Time evolution of statistical ensembles 68
3.2.1 *Liouville equation* 68
3.2.2 *Frobenius–Perron and Koopman operators* 69
3.2.3 *Boundary conditions* 70
3.3 Invariant measures 72
3.3.1 *Definition* 72
3.3.2 *Selection of an invariant measure* 73
3.3.3 *The basic invariant measures of Hamiltonian systems* 74
3.4 Correlation functions and spectral functions 75
3.5 Spectral theory on real frequencies 76
3.5.1 *Spectral decomposition on a Hilbert space* 76
3.5.2 *Purely discrete real spectrum* 77
3.5.3 *Continuous real spectrum* 78
3.5.4 *Continuous real spectrum and the Wiener–Khinchin theorem* 81
3.5.5 *Continuous real spectrum and Gaussian fluctuations* 82
3.6 Spectral theory on complex frequencies or resonance theory 83
3.6.1 *Analytic continuation to complex frequencies* 83
3.6.2 *Singularities as a spectrum of generalized eigenvalues* 87
3.6.3 *Definition of a trace* 91
3.7 Resonances of stationary points 94
3.7.1 *Trace formula and eigenvalues* 94
3.7.2 *Eigenstates and spectral decompositions* 96
3.7.3 *Hamiltonian stationary point of saddle type* 100
3.8 Resonances for hyperbolic sets with periodic orbits 103
3.8.1 *Trace formula* 103
3.8.2 *The Selberg–Smale Zeta function* 105
3.8.3 *Formulation of the eigenvalue problem* 110
3.8.4 *Fredholm determinant* 113
3.8.5 *Fredholm theory for the eigenstates* 114
3.8.6 *Periodic-orbit averages of observables* 116
3.9 Resonance spectrum at bifurcations 118

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Cambridge University Press
0521018250 - Chaos, Scattering and Statistical Mechanics
Pierre Gaspard
Frontmatter
More information

3.9.1 *Pitchfork bifurcation* 119
3.9.2 *Hopf bifurcation* 120
3.9.3 *Homoclinic bifurcation in a two-dimensional flow* 122
3.10 Liouvillian dynamics of one-dimensional maps 123

Chapter 4 **Probabilistic chaos** 126

4.1 Dynamical randomness and the entropy per unit time 126
4.1.1 *A model of observation* 127
4.1.2 *Information redundancy and algorithmic complexity* 128
4.1.3 *Kolmogorov–Sinai entropy per unit time* 130
4.2 The large-deviation formalism 131
4.2.1 *Separated subsets* 132
4.2.2 *Topological pressure and the dynamical invariant measures* 132
4.2.3 *Pressure functions based on the Lyapunov exponents* 135
4.2.4 *Entropy function and Legendre transform* 136
4.3 Closed hyperbolic systems 138
4.3.1 *The microcanonical measure as a Sinai–Ruelle–Bowen dynamical measure* 138
4.3.2 *The pressure function for closed systems* 140
4.3.3 *Generating functions of observables and transport coefficients* 141
4.4 Open hyperbolic systems 142
4.4.1 *The nonequilibrium invariant measure of the repeller* 143
4.4.2 *Connection with the dynamical invariant measure and the pressure function* 145
4.4.3 *Fractal repellers in two-degrees-of-freedom systems and their dimensions* 148
4.5 Generalized zeta functions 152
4.5.1 *Frobenius–Perron operators in the large-deviation formalism* 152
4.5.2 *The topological pressure as an eigenvalue* 154
4.6 Probabilistic Markov chains and lattice gas automata 156
4.6.1 *Markov chain models* 156
4.6.2 *Isomorphism between Markov chains and area-preserving maps* 157
4.6.3 *Repellers of Markov chains* 159
4.6.4 *Large-deviation formalism of Markov chains* 161

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Cambridge University Press
0521018250 - Chaos, Scattering and Statistical Mechanics
Pierre Gaspard
Frontmatter
More information

4.7 Special fractals generated by uniformly hyperbolic maps *163*
4.7.1 *Condition on the mean sojourn time in a domain* *163*
4.7.2 *Fractal repeller generated in trajectory reconstruction* *167*
4.8 Nonhyperbolic systems *169*

Chapter 5 **Chaotic scattering** *171*

5.1 Classical scattering theory *171*
5.1.1 *Motivations* *171*
5.1.2 *Classical scattering function and time delay* *172*
5.1.3 *The different types of trajectories* *174*
5.1.4 *Scattering operator for statistical ensembles* *176*
5.2 Hard-disk scatterers *176*
5.2.1 *Generalities* *176*
5.2.2 *The dynamics* *177*
5.2.3 *The Birkhoff mapping* *179*
5.2.4 *The one-disk scatterer* *180*
5.2.5 *The two-disk scatterer* *181*
5.2.6 *The three-disk scatterer* *183*
5.2.7 *The four-disk scatterer* *201*
5.3 Hamiltonian mapping of scattering type *210*
5.3.1 *Definition of the model* *210*
5.3.2 *Metamorphoses of the phase portraits* *211*
5.3.3 *Characteristic quantities of the chaotic repeller* *215*
5.4 Application to the molecular transition state *216*
5.4.1 *Model of photodissociation of* HgI_2 *216*
5.4.2 *Transition from a periodic to a chaotic repeller* *218*
5.4.3 *Three-branched Smale repeller and its characterization* *219*
5.5 Further applications of chaotic scattering *221*

Chapter 6 **Scattering theory of transport** *224*

6.1 Scattering and transport *224*
6.2 Diffusion and chaotic scattering *225*
6.2.1 *Large scatterers and the diffusion equation* *225*
6.2.2 *Escape-time function and escape rate* *226*
6.2.3 *Phenomenology of the escape process* *229*
6.2.4 *The escape-rate formula for diffusion* *231*
6.3 The periodic Lorentz gas *234*

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Pierre Gaspard
Frontmatter
More information

6.3.1 *Definition* 234
6.3.2 *The Liouville invariant measure* 235
6.3.3 *Finite and infinite horizons* 236
6.3.4 *Chaotic properties of the infinite Lorentz gas* 237
6.3.5 *The open Lorentz gas* 244
6.4 The multibaker mapping 250
6.4.1 *Definition* 250
6.4.2 *The Pollicott–Ruelle resonances and the escape-rate formula* 254
6.5 Escape-rate formalism for general transport coefficients 257
6.5.1 *General context* 257
6.5.2 *Transport coefficients and their Helfand moments* 258
6.5.3 *Generalization of the escape-rate formula* 261
6.6 Escape-rate formalism for chemical reaction rates 264
6.6.1 *Nonequilibrium thermodynamics of chemical reactions* 265
6.6.2 *The master equation approach* 266
6.7 Discussion 268
6.7.1 *Summary* 268
6.7.2 *Further applications of the escape-rate formalism* 269
6.7.3 *Relation to the thermostatted-system approach* 270
6.7.4 *The escape-rate formalism in the presence of external forces* 272

Chapter 7 **Hydrodynamic modes of diffusion** 275

7.1 Hydrodynamics from Liouvillian dynamics 275
7.1.1 *Historical background and motivation* 275
7.1.2 *Pollicott–Ruelle resonances and quasiperiodic boundary conditions* 276
7.2 Liouvillian dynamics for systems symmetric under a group of spatial translations 278
7.2.1 *Introduction* 278
7.2.2 *Suspended flows of infinite spatial extension* 279
7.2.3 *Assumptions on the properties of the mapping* 282
7.2.4 *Invariant measures* 283
7.2.5 *Time-reversal symmetry* 284
7.2.6 *The Frobenius–Perron operator on the infinite lattice* 284
7.2.7 *Spatial Fourier transforms* 285
7.2.8 *The Frobenius–Perron operators in the wavenumber subspaces* 286

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Pierre Gaspard
Frontmatter
More information

7.2.9 *Time-reversal symmetry for the* **k***-components* 288
7.2.10 *Reduction to the Frobenius–Perron operator of the mapping* 289
7.2.11 *Eigenvalue problem and zeta function* 289
7.2.12 *Consequences of time-reversal symmetry on the resonances* 291
7.2.13 *Relation to the eigenvalue problem for the flow* 292
7.3 Deterministic diffusion 293
7.3.1 *Introduction* 293
7.3.2 *Mean drift* 294
7.3.3 *The first derivative of the eigenstate with respect to the wavenumber* 295
7.3.4 *Diffusion matrix* 296
7.3.5 *Higher-order diffusion coefficients* 297
7.3.6 *Eigenvalues and the Van Hove function* 299
7.3.7 *Periodic-orbit formula for the diffusion coefficient* 302
7.3.8 *Consequences of the lattice symmetry under a point group* 303
7.4 Deterministic diffusion in the periodic Lorentz gas 305
7.4.1 *Properties of the infinite Lorentz gas* 305
7.4.2 *Diffusion and its dispersion relation* 309
7.4.3 *Cumulative functions of the eigenstates* 310
7.5 Deterministic diffusion in the periodic multibaker 312
7.5.1 *Properties of the periodic multibaker* 312
7.5.2 *The Frobenius–Perron operator and its Pollicott–Ruelle resonances* 313
7.5.3 *Generalized spectral decomposition* 316
7.5.4 *Analysis of the associated one-dimensional map* 318
7.5.5 *The root states of the two-dimensional map* 326
7.6 Extensions to the other transport processes 334
7.6.1 *Gaussian fluctuations of the Helfand moments* 334
7.6.2 *The minimal models of transport* 336
7.6.3 *Viscosity and self-diffusion in two-particle fluids* 337
7.6.4 *Spontaneous symmetry breaking and Goldstone hydrodynamic modes* 339
7.7 Chemio-hydrodynamic modes 340

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Pierre Gaspard
Frontmatter
More information

Chapter 8 **Systems maintained out of equilibrium** *343*

8.1 Nonequilibrium systems in Liouvillian dynamics *343*
8.2 Nonequilibrium steady states of diffusion *345*
8.2.1 *Phenomenological description of the steady states* *345*
8.2.2 *Deterministic description of the steady states* *346*
8.3 From the hydrodynamic modes to the nonequilibrium steady states *350*
8.3.1 *From the eigenstates to the nonequilibrium steady states* *350*
8.3.2 *Microscopic current and Fick's law* *352*
8.3.3 *Nonequilibrium steady states of the periodic Lorentz gas* *353*
8.3.4 *Nonequilibrium steady states of the periodic multibaker* *355*
8.3.5 *Nonequilibrium steady states of the Langevin process* *359*
8.4 From the finite to the infinite multibaker *361*
8.5 Generalization to the other transport processes *366*
8.6 Entropy production *368*
8.6.1 *Irreversible thermodynamics and the problem of entropy production* *370*
8.6.2 *Comparison with deterministic schemes* *371*
8.6.3 *Open systems and their Poisson suspension* *373*
8.6.4 *The ε-entropy* *376*
8.6.5 *Entropy production in the multibaker map* *378*
8.6.6 *Summary* *383*
8.7 Comments on far-from-equilibrium systems *385*

Chapter 9 **Noises as microscopic chaos** *387*

9.1 Differences and similarities between noises and chaos *387*
9.2 (ε, τ)-entropy per unit time *390*
9.2.1 *Dynamical processes* *390*
9.2.2 *Entropy of a process over a time interval T and a partition $\mathscr{C}$* *391*
9.2.3 *Partition (ε, τ)-entropy per unit time* *392*
9.2.4 *Cohen–Procaccia (ε, τ)-entropy per unit time* *393*
9.2.5 *Shannon–Kolmogorov (ε, τ)-entropy per unit time* *394*
9.3 Time random processes *397*
9.3.1 *Deterministic processes* *397*
9.3.2 *Bernoulli and Markov chains* *398*
9.3.3 *Birth-and-death processes* *399*
9.3.4 *Time-discrete, amplitude-continuous random processes* *402*

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Pierre Gaspard
Frontmatter
More information

9.3.5 *Time- and amplitude-continuous random processes* 406
9.3.6 *White noise* 411
9.3.7 *Lévy flights* 411
9.3.8 *Classification of the time random processes* 412
9.4 Spacetime random processes 415
9.4.1 *(ε, τ)-entropy per unit time and volume* 415
9.4.2 *Deterministic cellular automata* 415
9.4.3 *Lattice gas automata* 416
9.4.4 *Coupled map lattices* 416
9.4.5 *Nonlinear partial differential equations* 417
9.4.6 *Stochastic spin dynamics* 417
9.4.7 *Spacetime Gaussian fields* 417
9.4.8 *Sporadic spacetime random processes* 418
9.4.9 *Classification of spacetime random processes* 419
9.5 Random processes of statistical mechanics 419
9.5.1 *Ideal gases* 420
9.5.2 *The Lorentz gases and the hard-sphere gases* 424
9.5.3 *The Boltzmann–Lorentz process* 425
9.6 Brownian motion and microscopic chaos 429
9.6.1 *Hamiltonian and Langevin models of Brownian motion* 429
9.6.2 *A lower bound on the positive Lyapunov exponents* 430
9.6.3 *Some conclusions* 431

Chapter 10 **Conclusions and perspectives** 433

10.1 Overview of the results 433
10.1.1 *From dynamical instability to statistical ensembles* 433
10.1.2 *Dynamical chaos* 438
10.1.3 *Fractal repellers and chaotic scattering* 441
10.1.4 *Scattering theory of transport* 442
10.1.5 *Relaxation to equilibrium* 442
10.1.6 *Nonequilibrium steady states and entropy production* 447
10.1.7 *Irreversibility* 448
10.1.8 *Possible experimental support for the hypothesis of microscopic chaos* 451
10.2 Perspectives and open questions 452
10.2.1 *Extensions to general and dissipative dynamical systems* 453

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Pierre Gaspard
Frontmatter
More information

10.2.2 *Extensions in nonequilibrium statistical mechanics* *454*
10.2.3 *Extensions to quantum-mechanical systems* *456*

References *458*
Index *471*

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Pierre Gaspard
Frontmatter
More information

Preface

Today, there is a growing interest in understanding the role of chaos in nonequilibrium statistical mechanics. Although ergodic theory has been one of the seeds of modern dynamical systems theory, it is only recently that new methods have been developed – especially, in periodic-orbit theory – in order to quantitatively characterize the microscopic chaos as well as the intrinsic rates of decay or relaxation of statistical ensembles of trajectories. One of these intrinsic rates is the escape rate associated with the so-called fractal repeller which plays a central role in chaotic scattering. During recent years, chaotic scattering has been discovered in many different fields, from celestial mechanics and hydrodynamics to atomic, molecular, mesoscopic, and nuclear physics. In molecular systems, chaotic scattering provides a classical and statistical understanding of chemical reactions. Chaotic scattering is also closely related to transport processes like diffusion or viscosity. In this way, relationships can be established between the transport coefficients and the characteristic quantities of microscopic chaos, such as the Lyapunov exponents, the Kolmogorov–Sinai entropy, or the fractal dimensions. These results and their developments shed new light on nonequilibrium statistical mechanics and the problem of irreversibility.

The aim of the present book is to describe the theory of chaotic scattering and this new approach to nonequilibrium statistical mechanics starting from the principles of dynamical systems theory and from the hypothesis of microscopic chaos. For lack of space and time, the book only contains results on classical dynamical systems, although many fascinating and closely connected results have also been obtained in the context of quantum dynamics.

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This book is the outcome of several collaborations which I have had with my colleagues:

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