

# Contents

<i>Preface</i>	vii
1. *Introduction and outline	1
1.1 Hamiltonian dynamical systems approach to nonequilibrium statistical mechanics . . . . .	2
1.2 Thermostated dynamical systems approach to nonequilibrium statistical mechanics . . . . .	7
1.3 The red thread through this book . . . . .	11
<b>Part 1: Fractal transport coefficients</b>	<b>15</b>
2. *Deterministic diffusion	17
2.1 A simple model for deterministic diffusion . . . . .	17
2.2 A parameter-dependent fractal diffusion coefficient . . . . .	22
2.3 Summary . . . . .	28
3. Deterministic drift-diffusion	29
3.1 Drift-diffusion model: mathematical definition . . . . .	29
3.2 <sup>+</sup> Calculating deterministic drift and diffusion coefficients	32
3.2.1 Twisted eigenstate method . . . . .	33
3.2.2 Transition matrix methods . . . . .	37
3.2.3 Numerical comparison of the different methods . . . . .	39
3.3 The phase diagram . . . . .	40
3.4 Simple maps as deterministic ratchets . . . . .	49
3.5 *Summary . . . . .	54

4.	Deterministic reaction-diffusion	55
4.1	A reactive-diffusive multibaker map . . . . .	55
4.1.1	Deterministic models of reaction-diffusion . . . . .	56
4.1.2	The Frobenius-Perron operator . . . . .	60
4.2	Diffusive dynamics . . . . .	62
4.2.1	+Diffusive modes of the dyadic multibaker . . . . .	62
4.2.2	The parameter-dependent diffusion coefficient . . . . .	64
4.3	Reactive dynamics . . . . .	70
4.3.1	+Reactive modes of the dyadic multibaker . . . . .	70
4.3.2	The parameter-dependent reaction rate . . . . .	75
4.4	*Summary . . . . .	81
5.	Deterministic diffusion and random perturbations	83
5.1	Disordered dynamical systems . . . . .	83
5.2	Noisy dynamical systems . . . . .	89
5.3	*Summary . . . . .	98
6.	From normal to anomalous diffusion	99
6.1	Deterministic diffusion and bifurcations . . . . .	99
6.2	Anomalous diffusion in intermittent maps . . . . .	107
6.3	*Summary . . . . .	119
7.	From diffusive maps to Hamiltonian particle billiards	121
7.1	Correlated random walks in maps . . . . .	121
7.2	Correlated random walks in billiards . . . . .	128
7.3	*Summary . . . . .	134
8.	Designing billiards with irregular transport coefficients	137
8.1	Diffusion in the flower-shaped billiard . . . . .	137
8.2	+Random and correlated random walks . . . . .	141
8.3	Diffusion in porous solids . . . . .	148
8.4	*Summary . . . . .	150
9.	Deterministic diffusion of granular particles	153
9.1	Resonances and diffusion in the bouncing ball billiard . . . . .	153
9.2	+Diffusion by correlated random walks . . . . .	157
9.3	Vibratory conveyors . . . . .	160
9.4	*Summary . . . . .	161

<b>Part 2: Thermostated dynamical systems</b>	<b>163</b>
10. Motivation: coupling a system to a thermal reservoir	165
10.1 *Why thermostats? . . . . .	165
10.2 *Modeling thermal reservoirs: the Langevin equation . . .	167
10.3 Equilibrium velocity distributions for thermostated systems	173
10.4 Applying thermostats: the periodic Lorentz gas . . . . .	179
10.5 *Summary . . . . .	183
11. *The Gaussian thermostat	185
11.1 Construction of the Gaussian thermostat . . . . .	185
11.2 Chaos and transport in Gaussian thermostated systems .	189
11.2.1 Phase space contraction and entropy production .	189
11.2.2 Lyapunov exponents and transport coefficients . .	190
11.2.3 Nonequilibrium fractal attractors . . . . .	193
11.2.4 Electrical conductivity . . . . .	198
11.3 Summary . . . . .	202
12. The Nosé-Hoover thermostat	205
12.1 The dissipative Liouville equation . . . . .	205
12.2 Construction of the Nosé-Hoover thermostat . . . . .	208
12.2.1 Heuristic derivation . . . . .	208
12.2.2 Physics of this thermostat . . . . .	210
12.3 Properties of the Nosé-Hoover thermostat . . . . .	213
12.3.1 Chaos and transport . . . . .	213
12.3.2 +Generalized Hamiltonian formalism . . . . .	215
12.3.3 Fractals and transport . . . . .	218
12.4 +Subtleties of Nosé-Hoover dynamics . . . . .	222
12.4.1 Necessary conditions and generalizations . . . . .	222
12.4.2 Thermal reservoirs in nonequilibrium . . . . .	226
12.5 *Summary . . . . .	227
13. Universalities in Gaussian and Nosé-Hoover dynamics?	231
13.1 Non-Hamiltonian nonequilibrium steady states . . . . .	231
13.2 Phase space contraction and entropy production . . . . .	235
13.3 Transport coefficients and dynamical systems quantities .	240
13.4 Fractal attractors for nonequilibrium steady states . . . .	247
13.5 Nonlinear response in the driven periodic Lorentz gas . .	251

13.6	*Summary . . . . .	253
14.	Gaussian and Nosé-Hoover thermostats	257
14.1	Non-ideal Gaussian thermostat . . . . .	257
14.2	Non-ideal Nosé-Hoover thermostat . . . . .	261
14.3	+Further alternative thermostats . . . . .	264
14.4	*Summary . . . . .	266
15.	Stochastic and deterministic boundary thermostats	269
15.1	Stochastic boundary thermostats . . . . .	270
15.2	Deterministic boundary thermostats . . . . .	271
15.3	+Boundary thermostats from first principles . . . . .	273
15.4	Deterministic boundary thermostats for the driven peri- odic Lorentz gas . . . . .	279
15.4.1	Phase space contraction and entropy production . . . . .	280
15.4.2	Attractors, bifurcations and conductivity . . . . .	283
15.4.3	Lyapunov exponents . . . . .	286
15.5	Hard disk fluid under shear and heat flow . . . . .	287
15.5.1	Homogeneously and inhomogeneously driven shear and heat flows . . . . .	288
15.5.2	Shear and heat flows thermostated by determinis- tic scattering . . . . .	291
15.6	*Summary . . . . .	300
16.	Active Brownian particles and Nosé-Hoover dynamics	303
16.1	Brownian motion of migrating cells? . . . . .	304
16.2	+Moving biological entities as active Brownian particles . . . . .	306
16.3	+Bimodal velocity distributions and Nosé-Hoover dynamics . . . . .	308
16.4	*Summary . . . . .	314

## Part 3: Outlook and conclusions 317

17.	Further topics in chaotic transport theory	319
17.1	Fluctuation relations . . . . .	320
17.1.1	Entropy fluctuation in nonequilibrium steady states . . . . .	320
17.1.2	The Gallavotti-Cohen fluctuation theorem . . . . .	321
17.1.3	The Evans-Searles fluctuation theorem . . . . .	327
17.1.4	Jarzynski work relation and Crooks relation . . . . .	328

17.2	Lyapunov modes . . . . .	331
17.3	Fourier’s law . . . . .	337
17.3.1	The basic problem . . . . .	338
17.3.2	Heat conduction in anharmonic chaotic chains . . .	340
17.3.3	Heat conduction in chaotic particle billiards . . .	344
17.4	Pseudochaotic diffusion . . . . .	347
17.4.1	Microscopic chaos and diffusion? . . . . .	348
17.4.2	Polygonal billiard channels . . . . .	352
17.5	*Summary . . . . .	364
18.	*Conclusions . . . . .	367
18.1	Microscopic chaos and nonequilibrium statistical mechan- ics: the big picture . . . . .	367
18.2	Assessment of the main results . . . . .	371
18.2.1	Existence of fractal transport coefficients . . . . .	371
18.2.2	Universalities in thermostated dynamical systems? . . . . .	374
18.3	Important open questions . . . . .	376
18.3.1	Fractal transport coefficients . . . . .	377
18.3.2	Thermostated dynamical systems . . . . .	379
	Note added in proof . . . . .	380
	<i>Bibliography</i> . . . . .	381
	<i>Index</i> . . . . .	435