A Kinetic View of Statistical Physics

Pavel L. Krapivsky, Sidney Redner, and Eli Ben-Naim

February 21, 2010
Contents

Preface iii

Conventions v

1 APERITIFS 1
  1.1 Diffusion ................................................................. 1
  1.2 Single-Species Annihilation/Coalescence ........................... 4
  1.3 Two-Species Annihilation ............................................ 7

2 DIFFUSION 9
  2.1 The Probability Distribution ..................................... 9
  2.2 Central Limit Theorem .............................................. 11
  2.3 Walks with Broad Distributions .................................. 12
  2.4 Application to Gravity: The Holtsmark Distribution .......... 16
  2.5 First-Passage Properties ......................................... 19
  2.6 Exit Probabilities and Exit Times ............................... 22
  2.7 Reaction-Rate Theory .............................................. 27
  2.8 The Langevin Approach ............................................ 30
  2.9 Application to Surface Growth ................................... 32
  2.10 Problems ............................................................. 37

3 COLLISIONS 43
  3.1 Kinetic Theory ........................................................ 43
  3.2 The Lorentz Gas ...................................................... 46
  3.3 Lorentz Gas in an External Field .................................. 51
  3.4 Collisional Impact .................................................. 55
  3.5 Maxwell Molecules and Very Hard Particles ..................... 56
  3.6 Inelastic Gases ........................................................ 59
  3.7 Ballistic Agglomeration ............................................ 65
  3.8 Single-Lane Traffic ................................................ 67
  3.9 Problems ............................................................. 71

4 EXCLUSION 75
  4.1 Symmetric Exclusion Process ..................................... 75
  4.2 Asymmetric Exclusion Process ................................... 79
  4.3 Hydrodynamic Approach ........................................... 82
  4.4 Microscopic Approach .............................................. 86
  4.5 Open Systems ........................................................ 90
  4.6 Problems ............................................................. 95
## 5 Aggregation

5.1 The Master Equations .................................................. 99
5.2 Exact Solution Methods ............................................. 101
5.3 Gelation ..................................................................... 107
5.4 Scaling ....................................................................... 113
5.5 Aggregation with Input ............................................. 115
5.6 Exchange-Driven Growth ......................................... 121
5.7 Problems ................................................................. 124

## 6 Fragmentation

6.1 Binary Fragmentation .................................................. 127
6.2 Planar Fragmentation .................................................. 133
6.3 Reversible Polymerization ........................................ 137
6.4 Collisional Fragmentation .......................................... 141
6.5 Problems ................................................................. 144

## 7 Adsorption

7.1 Random Sequential Adsorption in One Dimension ........ 147
7.2 Phase Space Structure ................................................ 153
7.3 Adsorption in Higher Dimensions .............................. 158
7.4 Reversible Adsorption .............................................. 163
7.5 Polymer Translocation ............................................. 168
7.6 Problems ................................................................. 171

## 8 Spin Dynamics

8.1 Phenomenology of Coarsening ...................................... 173
8.2 The Voter Model .......................................................... 174
8.3 Ising-Glauber Model ................................................... 181
8.4 Mean-Field Approximation ..................................... 183
8.5 Glauber Dynamics in One Dimension ......................... 185
8.6 Glauber Dynamics in Higher Dimensions .................... 191
8.7 Spin-Exchange Dynamics ......................................... 195
8.8 Cluster Dynamics ...................................................... 199
8.9 Problems ................................................................. 203

## 9 Coarsening

9.1 Models ...................................................................... 205
9.2 Free Evolution ........................................................... 207
9.3 Case Studies in Non-Conservative Dynamics ................ 210
9.4 Final States ............................................................... 216
9.5 Defects ..................................................................... 217
9.6 Conservative Dynamics ........................................... 224
9.7 Extremal Dynamics ................................................... 228
9.8 Nucleation and Growth ............................................ 231
9.9 Problems ................................................................. 235

## 10 Disorder

10.1 Disordered Spin Chain ............................................... 240
10.2 Random Walk in a Random Potential ......................... 246
10.3 Random Walk in Random Velocity Fields ..................... 251
10.4 Problems ................................................................. 255
11 HYSTERESIS \hspace{1cm} 257
  11.1 Homogeneous Ferromagnets \hspace{1cm} 257
  11.2 Perturbation Analysis \hspace{1cm} 260
  11.3 Disordered Ferromagnets \hspace{1cm} 266
  11.4 Mean-field Model \hspace{1cm} 268
  11.5 Hysteresis in the Random-Field Ising Chain \hspace{1cm} 271
  11.6 Problems \hspace{1cm} 275

12 POPULATION DYNAMICS \hspace{1cm} 277
  12.1 Continuum Formulation \hspace{1cm} 277
  12.2 Discrete Reactions \hspace{1cm} 284
  12.3 Small Fluctuation Expansion \hspace{1cm} 290
  12.4 Large Fluctuations \hspace{1cm} 293
  12.5 Problems \hspace{1cm} 296

13 DIFFUSIVE REACTIONS \hspace{1cm} 301
  13.1 Role of the Spatial Dimension \hspace{1cm} 301
  13.2 The Trapping Reaction \hspace{1cm} 304
  13.3 Two-Species Annihilation \hspace{1cm} 308
  13.4 Single-Species Reactions in One Dimension \hspace{1cm} 310
  13.5 Reactions in Spatial Gradients \hspace{1cm} 318
  13.6 Problems \hspace{1cm} 324

14 COMPLEX NETWORKS \hspace{1cm} 327
  14.1 Non-Lattice Networks \hspace{1cm} 327
  14.2 Evolving Random Graphs \hspace{1cm} 328
  14.3 Random Recursive Trees \hspace{1cm} 334
  14.4 Preferential Attachment \hspace{1cm} 338
  14.5 Fluctuations in Networks \hspace{1cm} 341
  14.6 Problems \hspace{1cm} 345

Bibliography \hspace{1cm} 349
Preface

Statistical physics is an unusual branch of science. It is not defined by a specific subject *per se*, but rather by ideas and tools that work for an incredibly wide range of problems. Statistical physics is concerned with interacting systems that consist of a huge number of building blocks — particles, spins, agents, *etc.* The local interactions between these elements lead to emergent behaviors that can often be simple and clean, while the corresponding few-particle systems can exhibit bewildering properties that defy classification. From a statistical perspective, the large size of a system often plays an advantageous, not deleterious, role in leading to simple collective properties.

While the tools of equilibrium statistical physics are well-developed, the statistical description of systems that are out of equilibrium is less mature. In spite of more than a century of effort to develop a formalism for non-equilibrium phenomena, there still do not exist analogs of the canonical Boltzmann factor or the partition function of equilibrium statistical physics. Moreover, non-equilibrium statistical physics has traditionally dealt with small deviations from equilibrium. Our focus is on systems far from equilibrium, where conceptually simple and explicit results can be derived for their dynamical evolution.

Non-equilibrium statistical physics is perhaps best appreciated by presenting wide-ranging and appealing examples, and by developing an array of techniques to solve these systems. We have attempted to make our treatment self-contained, so that an interested reader can follow the text with a minimum of unresolved methodological mysteries or hidden calculational pitfalls. Our main emphasis is on exact analytical tools, but we also develop heuristic and scaling methods where appropriate. Our target audience is graduate students beyond their first year who have taken a graduate course in equilibrium statistical physics and have had a reasonable exposure to mathematical techniques. We also hope that this book will be accessible to students and researchers in computer science, probability theory and applied mathematics, quantitative biological sciences, and engineering, because a wide variety of phenomena in these fields also involve the time evolution of systems with many degrees of freedom.

We begin with a few “aperitifs” — an abbreviated account of some basic problems along with some hints at methods of solution. The next three chapters comprise the major theme of transport processes. Chapter 2 introduces random walks and diffusion phenomena, mechanisms that underlie much of non-equilibrium statistical physics. Next, we discuss collision-driven phenomena in chapter 3. We depart from the tradition of entirely focusing on the Boltzmann equation and its application to hydrodynamics. Instead, we emphasize pedagogically illuminating and tractable examples, such as the Lorentz gas and Maxwell models. In chapter 4, we give a brief overview of exclusion processes and the profound consequences that exclusion has on transport and the spatial distribution of particles.

The next three chapters discuss the kinetics of aggregation, fragmentation, and adsorption. The classic aggregation process — in which two clusters irreversibly merge to form a larger cluster — serves as a rich playground to illustrate exact solution methods and the emergence of scaling in cluster-size distributions. Many of these technical lessons will be applied throughout this book. Our presentation of the complementary process of fragmentation follows a similar logical development. We then treat the irreversible adsorption of extended objects onto a surface. Here a kinetic approach provides a remarkably easy way to solve the seemingly difficult geometric problem of determining the final coverage of the surface.

Chapters 8 & 9 are devoted to non-equilibrium spin systems. We first focus on kinetic Ising models because of their simplicity and their broad applicability to dynamic phenomena associated with phase transitions. The following chapter on coarsening develops a mesoscopic picture, in which the elemental degrees of freedom are droplets and interfaces, rather than the atomistic spins of the kinetic Ising model. These two viewpoints are complementary and each provides valuable insights. Chapter 10 gives a glimpse into the role of disorder
for three specific examples of non-equilibrium processes. The next chapter exploits the insights gained from studying spin systems and disorder to treat the phenomenon of hysteresis.

Chapters 12 & 13 are devoted to population dynamics and the kinetics of chemical reactions. The first of these two chapters highlights the role of discreteness. This feature can lead to time evolution that is much different than that predicted by the deterministic rate equations. The following chapter focuses on the essential role of spatial fluctuations and dimension-dependent effects on reaction kinetics. We close with a presentation of the master equation approach to understand basic properties of complex networks. As in the case of adsorption, the kinetic viewpoint leads to a powerful and intuitive way to determine many geometrical properties of networks.

We conclude each chapter with a short “Notes” section that provides a guide to additional reading. We direct the reader to books and review articles whenever possible. By this emphasis, we do not mean to slight original literature, but most relevant information can be found within these more comprehensive references. However, we do cite original sources when such an exposition is particularly useful pedagogically or when a particular subject has not yet been reviewed.

Our choice of topics has been guided by the desire to provide key ideas and core techniques that will help turn students of non-equilibrium statistical physics into practitioners. Due to space limitations as well as our own personal biases and lack of knowledge, many important topics have been omitted. We hope that a student who successfully studies from this book will then be ready to competently assimilate many other topics in non-equilibrium statistical physics by self study.

Although our coverage of topics is incomplete, the contained material is still too ambitious for a one-semester course. For such a course, we recommend most of chapter 2 (random walks/diffusion), the first three sections of chapter 3 (collisions), the first four sections of chapter 5 (aggregation), sections 7.1 & 7.4 in chapter 7, most of chapters 8 & 9 (spin systems and coarsening), the first two sections of chapter 12 (population dynamics), the first three sections of chapter 13 (diffusive reactions), and chapter 14 (complex networks). Students are encouraged to solve the problems; this is perhaps the most effective way to learn the material. In our experience, several sections and chapters are also well-suited for stand alone mini-courses and summer schools.

We owe a great debt of gratitude to numerous collaborators, colleagues, and students who have helped shape our thinking and who have also provided advice in the preparation of this book. Each of us has benefited from insights learned from long-term collaborators, and some of their insights have percolated their way into this book. We do not mention them by name because they are too numerous and we are sure to miss some. Nevertheless, we are truly grateful to them, and we are lucky to count many of these colleagues and co-authors among our friends.

We are grateful to many Boston University graduate students who enrolled in a course in non-equilibrium statistical physics that was based on material in this book and was taught by two of us (PLK and SR). Their questions and feedback on preliminary versions of chapters of this book have been extremely helpful. We especially thank Boston University students Luca D’Alessio, Kip Barros, and David Schaich for their careful reading of portions of the book and their helpful comments. We have also benefitted from the feedback of students in mini-courses based on this book at the NSF-sponsored Boulder Summer School and at the Perimeter Scholars Institute sponsored by the Perimeter Institute for Theoretical Physics. We thank our colleagues for reading early drafts of this book and for providing many useful suggestions and corrections. This includes Dani ben-Avraham, Harvey Gould, Jon Machta, and Mauro Mobilia. We are especially grateful to Kirone Mallick who read the entire book and provided numerous suggestions for improvements.

Two of the authors (PLK and SR) wish to thank the National Science Foundation for providing research funding over an extended period that helped in our writing of this book. EB is grateful to the Laboratory Directed Research and Development program at Los Alamos National Laboratory for continued support of his work. We would be grateful to receive errata and will maintain an up-to-date list of errata on our websites. Feel free to contact any of the authors: paulk@bu.edu (PLK), redner@bu.edu (SR), or ebn@lanl.gov (EB).

* * * * * * * * *

PLK thanks Genja, Lyuba, Dana, and other members of his family for things that have nothing to do with statistical physics. SR thanks his children Rebecca and Gabriel, and his wife Anita, for their forebearance, support, and love during the preparation of this book. EB thanks his loving family, Ellen, Micha, Daniel, and Talia, for everything.