## Contents

Preface		page 5
1	FIRST PASSAGE FUNDAMENTALS	7
1.1	What is a First-Passage Process?	7
1.1.1	A Simple Illustration	7
1.1.2	Fundamental Issues	8
1.2	Connection between First-Passage and Occupation Probabilities	9
1.3	Probability Distribution of a One-Dimensional Random Walk	11
1.3.1	Discrete Space and Time	11
1.3.2	Discrete Space and Continuous Time	13
1.3.3	Continuous Space and Time	15
1.4	Relation between Laplace Transforms and Real Time Quantities	18
1.5	Asymptotics of the First-Passage Probability	20
1.6	Connection between First-Passage and Electrostatics	22
1.6.1	Background	22
1.6.2	The Green's Function Formalism	23
1.6.3	Laplacian Formalism	25
1.7	Random Walks and Resistor Networks	28
1.7.1	Introduction	28
1.7.2	The Basic Relation	28
1.7.3	Escape Probability, Resistance, and Pólya's Theorem	30
1.8	Epilogue	31
2	FIRST PASSAGE IN AN INTERVAL	32
2.1	Introduction	32
2.1.1	Basic Questions	32
2.2	Time-Dependent Formulation	33
2.2.1	Survival Probability: Absorption Mode	33
2.2.2	First-Passage Probability and Mean Exit Times	36
2.3	Time Integrated Formulation	44
2.3.1	Splitting Probabilities and Unconditional Exit Time: Absorption Mode	44
2.3.2	Conditional Mean Exit Times: Absorption Mode	50
2.3.3	Transmission Mode	52
2.3.4	Biased Diffusion as a Singular Perturbation	53
2.4	Discrete Space Random Walk	55
2.4.1	Illustration for a Short Chain	55
2.4.2	First-Passage Probabilities	57
2.4.3	Mean First-Passage Time	61
3	SEMI-INFINITE SYSTEM	63
3.1	The Basic Dichotomy	63

3.2	Image Method	63
3.2.1	The Concentration Profile	63
3.2.2	First-Passage Properties	65
3.3	Systematic Approach	72
3.3.1	The Green's Function Solution	72
3.3.2	Constant-Density Initial Condition	73
3.4	Discrete Random Walk	75
3.4.1	The Reflection Principle	75
3.4.2	Consequences for First Passage	75
3.4.3	Origin Crossing Statistics	77
3.5	Imperfect Absorption	81
3.5.1	Motivation	81
3.5.2	Radiation Boundary Condition	82
3.5.3	Connection to a Composite Medium	84
3.5.4	Equivalence to the Radiation Boundary Condition	87
3.6	The Quasi-Static Approximation	87
3.6.1	Motivation	87
3.6.2	Quasi-Static Solution at an Absorbing Boundary	88
3.6.3	Quasi-Static Solution at a Radiation Boundary	88
4	ILLUSTRATIONS OF FIRST PASSAGE IN SIMPLE GEOMETRIES	90
4.1	First Passage in Real Systems	90
4.2	Neuron Dynamics	91
4.2.1	Some Basic Facts	91
4.2.2	Integrate-and-Fire Model	91
4.3	Self-Organized Criticality	93
4.3.1	Isotropic and Directed Sandpile Models	94
4.3.2	Bak-Sneppen Model	95
4.3.3	Related Systems	99
4.4	Kinetics of Spin Systems	101
4.4.1	Background	101
4.4.2	Solution to the One-Dimensional Ising-Glauber Model	102
4.4.3	Solution to the Voter Model in all Dimensions	104
4.5	First Passage in Composite and Fluctuating Systems	106
4.5.1	Motivation	106
4.5.2	Segments with Different Diffusivities	106
4.5.3	Segments with Different Bias Velocities	108
4.5.4	Resonant First Passage in a Fluctuating Medium	111
4.6	Interval with Spatially Variable Diffusion	114
4.6.1	Basic Examples	114
4.6.2	Diffusivity $1 - (x/N)^2$	114
4.6.3	Diffusivity $1 -  x /N$	115
4.6.4	Diffusivity $(1 -  x /N)^{\mu}$	116
4.7	The Expanding Cage	117
4.7.1	General Considerations	117
4.7.2	Slowly Expanding Cage: Adiabatic Approximation	117
4.7.3	Rapidly Expanding Cage: Free Approximation	118
4.7.4	Marginally Expanding Cage	118
4.7.5	Iterated Logarithm Law for Ultimate Survival	121
4.8	The Moving Cliff	122
4.8.1	Rapidly Moving Cliff	122

 $\mathbf{2}$ 

4.8.2	Marginally Moving Cliff	123
4.8.3	Diffusing Cliff	125
5	FRACTAL AND NON-FRACTAL NETWORKS	127
5.1	Beyond One Dimension	127
5.2	Cayley Tree	128
5.3	Hierarchical Three-Tree	130
5.3.1	Transmission in the First-Order Tree	130
5.3.2	Exact Renormalization for the $N^{\text{th}}$ -Order Tree	131
5.3.3	Reflection in the Three-Tree	134
5.3.4	Conclusion	136
5.4	Comb Structures	136
5.4.1	Introduction	136
5.4.2	Homogeneous Comb	137
5.4.3	Hierarchical Comb	142
5.5	Hydrodynamic Transport	145
5.5.1	Single-Sidebranch Network	146
5.5.2	Single-Junction Network	149
5.5.3	The Hierarchical Blob	150
6	SYSTEMS WITH SPHERICAL SYMMETRY	156
6.1	Introduction	156
6.2	First Passage between Concentric Spheres	156
6.2.1	Splitting Probabilities	156
6.2.2	First Passage to a Sphere in Radial Potential Flow	158
6.2.3	Connection between Diffusion in General Dimension and Radial Drift in Two Dimensions	160
6.3	First Passage to a Sphere	161
6.3.1	Image Solution	161
6.3.2	Efficient Simulation of Diffusion-Limited Aggregation	162
6.4	Time-Dependent First-Passage Properties	164
6.4.1	Overview	164
6.4.2	Both Boundaries Absorbing	164
6.4.3	One Reflecting and One Absorbing Boundary	165
6.5	Reaction Rate Theory	167
6.5.1	Background	167
6.5.2	Time-Dependent Solution for General $d$	168
6.5.3	Elementary Time-Dependent Solution for $d = 3$	170
6.5.4	Quasi-Static Approach	171
6.5.5	Closest Particle to an Absorbing Sphere	172
7	WEDGE DOMAINS	175
7.1	Why Study the Wedge?	175
7.2	Two-Dimensional Wedge	176
7.2.1	Solution to the Diffusion Equation	176
7.2.2	Physical Implications	177
7.3	Three-Dimensional Cone	179
7.4	Conformal Transformations and Electrostatic Methods	180
7.4.1	Point Source and Line Sink	181
7.4.2	General Wedge Angles	182
7.5	First-Passage Times	184
7.5.1	Infinite Two-Dimensional Wedge	184
7.5.2	Pie Wedge in Two Dimensions	185
7.5.3	Infinite Three-Dimensional Cone	186

3

7.5.4	Conditional Exit Time for the Infinite Wedge	186
7.6	Extension to Time-Dependent First-Passage Properties	186
8	APPLICATIONS TO SIMPLE REACTIONS	188
8.1	Reactions as First-Passage Processes	188
8.2	Kinetics of the Trapping Reaction	189
8.2.1	Exact Solution in One Dimension	190
8.2.2	Lifshitz Argument for General Spatial Dimension	193
8.3	Reunions and Reactions of Three Diffusing Particles	195
8.3.1	Prey Survival Probability	196
8.3.2	Pair Meeting Probabilities	198
8.3.3	Lead and Order Probabilities	199
8.3.4	Extension to Arbitrary Number of Particles	201
8.4	Diffusion-Controlled Reactions	203
8.4.1	Basic Properties	203
8.4.2	The Capture Reaction, $p + P \rightarrow P$	203
8.4.3	Coalescence, $A + A \rightarrow A$	207
8.4.4	Annihilation, $A + A \rightarrow 0$	209
8.4.5	Aggregation, $A_i + A_k \rightarrow A_{i+j}$	211
8.5	Ballistic Annihilation	214
8.5.1	Two-Velocity Model	215
8.5.2	Three-Velocity Model	217
References		220
Index	<u>c</u>	227

## Preface

You arrange a 7pm date at a local bistro. Your punctual date arrives at 6:55, waits until 7:05, concludes that you will not show up, and leaves. At 7:06, you saunter in – "just a few minutes" after 7 (see Cover). You assume that you arrived first and wait for your date. The wait drags on and on. "What's going on?" you think to yourself. By 9pm, you conclude that you were stood up, return home, and call to make amends. You explain, "I arrived around 7 and waited 2 hours! My probability of being at the bistro between 7 and 9pm, P(bistro, t), was nearly one! How did we miss each other?" Your date replies, "I don't care about your occupation probability. What mattered was your first-passage probability, F(bistro, t), which was zero at 7pm. GOOD BYE!" Click!

The moral of this juvenile parable is that first passage underlies many stochastic processes, in which the event, such as a dinner date, a chemical reaction, the firing of a neuron, or the triggering of a stock option, relies on a variable reaching a specified value *for the first time*. In spite of the wide applicability of first-passage phenomena (or perhaps because of it), there does not seem to be a pedagogical source on this topic. For those with a serious interest, essential information is scattered and presented at diverse technical levels. In my attempts to learn the subject, I also encountered the proverbial conundrum that a fundamental result is "well-known to (the vanishingly small subset of) those who know it well".

In response to this frustration, I attempt to give a unified presentation of first-passage processes and illustrate some of its beautiful and fundamental consequences. My goal is to help those with modest backgrounds learn essential results quickly. The intended audience is physicists, chemists, mathematicians, engineers, and other quantitative scientists. The technical level should be accessible to the motivated graduate student.

My literary inspirations for this book include Random Walks and Electric Networks, by P. G. Doyle and J. L. Snell (Carus Mathematical Monographs #22, Mathematical Association of America, Washington, D. C.,1984), which cogently describes the relation between random walks and electrical networks, and A Primer on Diffusion Problems, by R. Ghez (Wiley, 1988) which gives a nice exposition of solutions to physically-motivated diffusion problems. This book is meant to complement classic monographs, such as An Introduction to Probability Theory and its Applications, by W. Feller (Wiley, New York, 1968), Aspects and Application of the Random Walks, by G. H. Weiss, (North-Holland, Amsterdam, 1996), and Stochastic Processes in Physics and Chemistry, by N. G. van Kampen (North-Holland, Amsterdam, 1997). Each of these very worthwhile books discusses first-passage phenomena, but secondarily rather than as a comprehensive overview.

I begin with fundamental background in Chap. 1 and outline the relation between occupation and firstpassage probabilities, as well as the connection between first passage and electrostatics. Many familiar results from electrostatics can be easily adapted to give first-passage properties in the same geometry. In Chap. 2, I discuss first passage in a one-dimensional interval. This provides a simple laboratory for answering basic questions, such as: What is the probability that a diffusing particle eventually exits at either end? How long does it take to exit? These problems are solved both by direct approaches and by developing the electrostatic equivalence. Chapter 3 treats first passage in a semi-infinite interval both by standard approaches and by the familiar image method. I also discuss surprising consequences of the basic dichotomy between certain return to the starting point and infinite mean return time.

Chapter 4 is devoted to illustrations of the basic theory. I discuss neuron dynamics, realizations of self-

## Preface

organized criticality, and the dynamics of spin systems. These all have the feature that they can be viewed as first-passage processes in one dimension. I also treat stochastic resonant escape from fluctuating and inhomogeneous media, for which the time-independent electrostatic formalism provides a relatively easy way to solve for mean first-passage times. Finally, I discuss the survival of a diffusing particle in a growing "cage" and near a moving "cliff", where particularly rich behavior arises when diffusion and the motion of the boundary have the same time dependence.

In Chap. 5, I turn to first passage on branched, self-similar structures. I emphasize self-similar systems because this feature allows us to solve for the first-passage probability by renormalization. Another essential feature of branched systems is the competition between transport along the "backbone" from source to sink and detours along sidebranches. I give examples that illustrate this basic competition and the transition from scaling, in which a single time scale accounts for all moments of the first-passage time, to multiscaling, in which each moment is governed by a different time scale.

I then treat spherically-symmetric geometries in Chap. 6 and discuss basic applications, such as efficient simulations of diffusion-limited aggregation and the Smoluchowski chemical reaction rate. First passage in wedge and conical domains are presented in Chap. 7. I discuss how the wedge geometry can be solved elegantly by the mapping to electrostatics and conformal transformations. These systems provide the kernel for understanding the main topic of Chap. 8, namely, the kinetics of one-dimensional diffusion-controlled reactions. This includes trapping, the reactions among three diffusing particles on the line, as well as basic bimolecular reactions, including capture  $p + P \rightarrow P$ , annihilation  $A + A \rightarrow 0$ , coalescence  $A + A \rightarrow A$ , and aggregation  $A_i + A_j \rightarrow A_{i+j}$ . The chapter ends with a brief treatment of ballistic annihilation.

A large fraction of this book discusses either classical first-passage properties or results about first passage from contemporary literature, but with some snippets of new results sprinkled throughout. However, several topics are either significant extensions of published results or are original. This includes the time-integrated formalism to compute the first-passage time in fluctuating systems (Section 4.5), aspects of survival in an expanding interval (Section 4.7), return probabilities on the hierarchical tree and homogeneous comb (Sections 5.3 & Subsection 5.4.2), the first-passage probability on the hierarchical blob (Section 5.5), and reactions of three diffusing particles on the line (Section 8.3).

This book has been influenced by discussions or collaborations with Dani ben-Avraham, Eli Ben-Naim, Charlie Doering, Laurent Frachebourg, Slava Ispolatov, Joel Koplik, Paul Krapivsky, Satya Majumdar, Francois Leyvraz, Michael Stephen, George Weiss, David Wilkinson, and Bob Ziff to whom I am grateful for their friendship and insights. I thank Bruce Taggart of the U.S. National Science Foundation for providing financial support at a crucial juncture in the writing, as well as Murad Taqqu and Mal Teich for initial encouragement. Elizabeth Sheld helped me get this project started with her invaluable organizational assistance. I also thank Satya Majumdar for advice on a preliminary manuscript and Erkki Hellén for a critical reading of a nearly final version. I am especially indebted to Paul Krapivsky, my next-door neighbor for most of the past 6 years, for many pleasant collaborations and for much helpful advice. While it is a pleasure to acknowledge the contributions of my colleagues, errors in presentation are mine alone.

Even in the final stages of writing, I am acutely aware of many shortcomings in my presentation. If I were to repair them all, I might never finish. This book is still work "in progress" and I look forward to receiving your corrections, criticisms, and suggestions for improvements (redner@bu.edu).

Finally and most importantly, I thank my family for their love and constant support and for affectionately tolerating me while I was writing this book.