

CONTENTS

I. Theoretical Foundations	1
<i>by P. Grigolini</i>	
II. Basic Description of the Rules Leading to the Adiabatic Elimination of Fast Variables	29
<i>by P. Grigolini and F. Marchesoni</i>	
III. Continued Fractions in the Theory of Relaxation	81
<i>by G. Grosso and G. Pastori Parravicini</i>	
IV. Memory Function Methods in Solid State Physics	133
<i>by G. Grosso and G. Pastori Parravicini</i>	
V. Molecular Dynamics: Intense External Fields	183
<i>by M. W. Evans</i>	
VI. Nonlinear Effects in Molecular Dynamics of the Liquid State	225
<i>by M. Ferrario, P. Grigolini, A. Tani, R. Vallauri, and B. Zambon</i>	
VII. Dynamical Properties of Hydrogen-Bonded Liquids	277
<i>by D. Bertolini, M. Cassetari, M. Ferrario, P. Grigolini, and G. Salvetti</i>	
VIII. Slow Motion EPR Spectra in Terms of a Generalized Langevin Equation	321
<i>by M. Giordano, P. Grigolini, D. Leporini, and P. Marin</i>	
IX. The Theory of Chemical Reaction Rates	389
<i>by T. Fonseca, J. A. N. F. Gomes, P. Grigolini, and F. Marchesoni</i>	

X.	Experimental Investigation on the Effect of Multiplicative Noise by Means of Electric Circuits	445
	<i>by S. Faetti, C. Festa, L. Fronzoni, and P. Grigolini</i>	
XI.	Interdisciplinary Subjects (Population Genetics): The Time Properties of a Model of Random Fluctuating Selection	477
	<i>by P. Grigolini, F. Marchesoni, and S. Presciuttini</i>	
XII.	Stochastic Processes in Astrophysics: Stellar Formation and Galactic Evolution	493
	<i>by F. Ferrini, F. Marchesoni, and S. N. Shore</i>	
	Author Index	531
	Subject Index	543

I

THEORETICAL FOUNDATIONS

P. GRIGOLINI

CONTENTS

I.	Introduction	1
II.	The Zwanzig Projection Technique	4
III.	The Mori Projection Technique	10
IV.	Molecular Dynamics: A Challenge to the Fokker-Planck and Langevin Approaches	24
V.	Concluding Remarks	26
	References	26

II

BASIC DESCRIPTION OF THE RULES LEADING TO THE ADIABATIC ELIMINATION OF FAST VARIABLES

P. GRIGOLINI and F. MARCHESONI

CONTENTS

I.	Introduction	29
II.	An Illustrative Example to Make Readers Familiar with the AEP	34
III.	The Basic Rules for a Systematic Expansion	43
IV.	More on the Illustrative Example of Section II	50
V.	Applications to Effective Liouvillians	61
	A. One-Dimensional Stochastic Differential Equation of the Langevin Type	63
	B. Two-Dimensional Stochastic Differential Equation of the Langevin Type	66
VI.	Rotational Brownian Motion	70
VII.	On the Choice of the Best Projection Operator	73
VIII.	Concluding Remarks	77
	References	78

III

CONTINUED FRACTIONS IN THE THEORY OF RELAXATION

G. GROSSO and G. PASTORI PARRAVICINI

CONTENTS

I.	Introduction	81
II.	Continued Fractions: Definitions and Basic Algebraic Properties	82
III.	Elementary Analytic Properties of Continued Fractions	85
IV.	Relation between Power Series and Continued Fractions	91
V.	Relation between Green's Function and Continued Fractions	96
	A. Introductory Remarks	96
	B. The Classical Moment Problem	100
	C. The Relaxation Moment Problem	103
VI.	Product-Difference Recursion Algorithms	104
VII.	Properties of Orthogonal Polynomials	110
	A. Definitions and Basic Properties	110
	B. Relation between Orthogonal Polynomials and Continued Fractions	116
	C. Orthogonal Polynomials and Modified Moments	122
VIII.	Error Bounds and Continued Fractions	124
	References	130

IV

MEMORY FUNCTION METHODS IN SOLID STATE PHYSICS

G. GROSSO and G. PASTORI PARRAVICINI

CONTENTS

I.	Introduction	133
II.	Representation of Model Hamiltonians in a Local Basis	135
III.	Memory Function Methods	139
	A. The Moment Method	139
	B. The Lanczos Method	142
	C. The Recursion Method	146
	D. Projective Techniques and the Memory Function Formalism	149
IV.	Asymptotic Behavior of Continued-Fraction Coefficients	159
V.	Application of Memory Function Methods in Periodic and Aperiodic Solids	163
	A. Introductory Remarks	163
	B. Green's Function Formulation of the Impurity Problem	163
	C. The Recursion Method for the Localized and Extended Impurity Problem: Applications and Perspectives	167
VI.	Electrons in Lattices with Stochastic Disorder	171
	A. Introductory Remarks and Diagonal Disorder	171
	B. Coherent Potential Approximation and the Recursion Method	174
	C. Localization and Spectra of Disordered Systems	177
	References	178

MOLECULAR DYNAMICS: INTENSE EXTERNAL FIELDS

M. W. EVANS

CONTENTS

I.	Historical Development	183
II.	Computer Simulation	188
	A. Basic Techniques	189
	1. Polarizability and Hyper polarizability	195
	B. Nonlinear Molecular Dynamics under Intense Force Fields	198
	C. Transients Induced by Alternating Fields	200
III.	Analysis of the Numerical Data with RMT	202
	A. The Decoupling Effect	202
	1. Decoupling Effects in the Quasi-Markov Limit	203
	B. Deexcitation Effects	206
	1. Linear and Nonlinear Systems Far from Equilibrium	206
	2. Comparison with Computer Simulation	209
IV.	Field Effects in Chiral Molecules: Computer Simulation	212
	A. Rise and Fall Transients in Fluorochloroacetonitrile	220
	1. Rototranslational Correlations in the Laboratory Frame of Reference	221
	Acknowledgments	222
	References	222

VI

NONLINEAR EFFECTS IN MOLECULAR DYNAMICS OF THE LIQUID STATE

M. FERRARIO, P. GRIGOLINI, A. TANI, R. VALLAURI, and
B. ZAMBON

CONTENTS

I.	Introduction	225
II.	Linear One-Dimensional System and the RMT	227
III.	Computer Simulation of a One-Dimensional Lennard-Jones System	233
	A. The System	233
	B. The Algorithm	234
	C. Check of the Equilibrium Properties	235
	D. Standard Observations in Molecular Dynamics	237
	E. Results of an Excitation Experiment	239
IV.	The Effective Nonlinear Potential	241
V.	The Nonlinear Itinerant Oscillator	246
VI.	Rotation Dynamics: Computer Simulation of Equilibrium and Nonequilibrium Properties	261
	A. Computational Details	262
	B. Results	263
	C. Excited Initial Distribution and Corresponding Angular Velocity Correlation Function	269
	D. The Excitation	270
VII.	Concluding Remarks	274
	References	275

VII

DYNAMICAL PROPERTIES OF HYDROGEN-BONDED LIQUIDS

D. BERTOLINI, M. CASSETTARI, M. FERRARIO,
P. GRIGOLINI, and G. SALVETTI

CONTENTS

I.	Introduction	277
II.	Hydrogen-Bond Definition and Statistics	280
III.	Hydrogen-Bond Dynamics	284
IV.	The RMT at Work: Long-Time Behavior Taking Hydrogen-Bond Dynamics into Account	286
V.	Parameters of Hydrogen-Bond Dynamics	292
	A. Calculation of the Probability p_B	294
	B. The Hydrogen-Bond Lifetime τ_{HB}	298
VI.	Dielectric Relaxation	300
VII.	Translational Diffusion	304
VIII.	Non-Gaussian Properties as an Effect of the H-Bond Dynamics	309
IX.	The Dynamics of Other Hydrogen-Bonded Liquids	314
	A. D_2O	314
	B. Alcohols	315
X.	Concluding Remarks	317
	References	318

VIII

SLOW MOTION EPR SPECTRA IN TERMS OF A GENERALIZED LANGEVIN EQUATION

M. GIORDANO, P. GRIGOLINI, D. LEPORINI,
and P. MARIN

CONTENTS

I. Introduction	321
II. General Theory	326
III. Applications	334
A. Hyperfine Structure ($S = 1/2$, $I = 1$)	335
B. Zero Field Splitting ($S = 1$)	348
1. Evolution of the Moments	349
2. Analytical Structure	351
C. Isolated Paramagnetic Ions with Large Anisotropy (Cu^{2+} : $S = 1/2$, $I = 3/2$)	357
D. ESR Lineshapes in the Presence of an Orienting Potential	361
1. Axial g-Splitting Tensor ($S = 1/2$)	362
2. Zero Field Splitting ($S = 1$)	366
3. Hyperfine Interaction ($S = 1/2$, $I = 1$; $S = 1/2$, $I = 3/2$)	367
E. Inertial Effects on the ESR Lineshape	372
IV. Final Remarks	377
Appendix A	378
Appendix B	385
References	387

IX

THE THEORY OF CHEMICAL REACTION RATES*

T. FONSECA, J. A. N. F. GOMES, P. GRIGOLINI, and
F. MARCHESONI

CONTENTS

I.	Motivation	389
II.	The Kramers Model and its Extensions	392
	A. The Kramers Model	393
	B. The Bistable Model and Other Generalizations of the Kramers Method	397
III.	Multimodal Theories	400
	A. Two Detailed Models	401
	B. The Coupled Double-Well Oscillator	402
IV.	Non-Markovian Effects on the Rate	411
	A. Noise-Activated Escape Rate in the Presence of Memory Effects	411
	1. Examples of Non-Markovian External Noises	412
	2. Chemical Reactions Driven by Bona Fide Non-Markovian Fluctuation- Dissipation Processes	417
	B. Activation of a Chemical Reaction Process via Electromagnetic Excitation	425
V.	Discussion and General Perspective	429
	A. Supporting Experimental Evidence	430
	B. Settled and Unsettled Problems in the Field of Chemical Reaction Rate Theory	432
	References	440

X

EXPERIMENTAL INVESTIGATION ON THE EFFECT OF MULTIPLICATIVE NOISE BY MEANS OF ELECTRIC CIRCUITS

S. FAETTI, C. FESTA, L. FRONZONI, and P. GRIGOLINI

CONTENTS

I.	Introduction	445
II.	Review of Experimental Research	450
III.	Experimental Apparatus	453
	A. The Analog Circuit	453
	B. The Noise Source	455
IV.	Fluctuating Double-Well Potential: A Comparison of Theory and Experiment	457
	A. The Case of a Purely Multiplicative Noise: Equilibrium Distribution	460
	B. The Influence of Additive Noise and Inertia on Equilibrium Properties	461
V.	Concluding Remarks and Perspective on Further Investigative Work	470
	References	474

XI

INTERDISCIPLINARY SUBJECTS (POPULATION GENETICS): THE TIME PROPERTIES OF A MODEL OF RANDOM FLUCTUATING SELECTION

P. GRIGOLINI, F. MARCHESONI, and S. PRESCIUTTINI

CONTENTS

I. Introduction	477
II. A Detailed Model for Stochastic Selection	480
III. The Time Needed to Reach a New Distribution of Gene Frequencies and Their Equilibrium Density	485
IV. Concluding Remarks	489
Acknowledgments	490
References	491

XII

**STOCHASTIC PROCESSES IN
ASTROPHYSICS:
STELLAR FORMATION AND
GALACTIC EVOLUTION**

F. FERRINI, F. MARCHESONI, and S. N. SHORE

CONTENTS

I. Introduction	493
II. Agglomeration Phenomena (Coagulation Equation Applications)	495
A. Solar System Formation	495
B. Star Formation—Initial Mass Function	497
III. Percolation Models	502
IV. Langevin Systems and the Fokker-Planck Equation	504
V. Mathematical Treatment of a Simple Astrophysical Model	517
References	526