C. W. Gardiner

# Handbook of Stochastic Methods

## for Physics, Chemistry and the Natural Sciences

**Third Edition**
**With 30 Figures**

Springer

# Contents


**1. A Historical Introduction** . . . 1
1.1 Motivation . . . 1
1.2 Some Historical Examples . . . 2
1.2.1 Brownian Motion . . . 2
1.2.2 Langevin's Equation . . . 6
1.3 Birth-Death Processes . . . 8
1.4 Noise in Electronic Systems . . . 11
1.4.1 Shot Noise . . . 11
1.4.2 Autocorrelation Functions and Spectra . . . 15
1.4.3 Fourier Analysis of Fluctuating Functions: Stationary Systems . . . 17
1.4.4 Johnson Noise and Nyquist's Theorem . . . 18

2. **Probability Concepts** . . . 21
2.1 Events, and Sets of Events . . . 21
2.2 Probabilities . . . 22
2.2.1 Probability Axioms . . . 22
2.2.2 The Meaning of *P(A)* . . . 23
2.2.3 The Meaning of the Axioms . . . 23
2.2.4 Random Variables . . . 24
2.3 Joint and Conditional Probabilities: Independence . . . 25
2.3.1 Joint Probabilities . . . 25
2.3.2 Conditional Probabilities . . . 25
2.3.3 Relationship Between Joint Probabilities of Different Orders 26
2.3.4 Independence . . . 27
2.4 Mean Values and Probability Density . . . 28
2.4.1 Determination of Probability Density by Means of Arbitrary Functions . . . 28
2.4.2 Sets of Probability Zero . . . 29
2.5 Mean Values . . . 29
2.5.1 Moments, Correlations, and Covariances . . . 30
2.5.2 The Law of Large Numbers . . . 30
2.6 Characteristic Function . . . 32
2.7 Cumulant Generating Function: Correlation Functions and Cumulants 33
2.7.1 Example: Cumulant of Order 4: $((\hat{X}_i X \hat{})$ . . . 35
2.7.2 Significance of Cumulants . . . 35
2.8 Gaussian and Poissonian Probability Distributions . . . 36
2.8.1 The Gaussian Distribution . . . 36

2.8.2 Central Limit Theorem . . . 37
2.8.3 The Poisson Distribution . . . 38
2.9 Limits of Sequences of Random Variables . . . 39
2.9.1 Almost Certain Limit . . . 40
2.9.2 Mean Square Limit (Limit in the Mean) . . . 40
2.9.3 Stochastic Limit, or Limit in Probability . . . 40
2.9.4 Limit in Distribution . . . 41
2.9.5 Relationship Between Limits . . . 41

**3. Markov Processes** . . . 42
3.1 Stochastic Processes . . . 42
3.2 Markov Process . . . 43
3.2.1 Consistency—the Chapman-Kolmogorov Equation . . . 43
3.2.2 Discrete State Spaces . . . 44
3.2.3 More General Measures . . . 44
3.3 Continuity in Stochastic Processes . . . 45
3.3.1 Mathematical Definition of a Continuous Markov Process . 46
3.4 Differential Chapman-Kolmogorov Equation . . . 47
3.4.1 Derivation of the Differential Chapman-Kolmogorov Equation . . . 48
3.4.2 Status of the Differential Chapman-Kolmogorov Equation . 51
3.5 Interpretation of Conditions and Results . . . 51
3.5.1 Jump Processes: The Master Equation . . . 52
3.5.2 Diffusion Processes—the Fokker-Planck Equation . . . 52
3.5.3 Deterministic Processes—Liouville's Equation . . . 53
3.5.4 General Processes . . . 54
3.6 Equations for Time Development in Initial Time—Backward Equations . . . 55
3.7 Stationary and Homogeneous Markov Processes . . . 56
3.7.1 Ergodic Properties . . . 57
3.7.2 Homogeneous Processes . . . 60
3.7.3 Approach to a Stationary Process . . . 61
3.7.4 Autocorrelation Function for Markov Processes . . . 64
3.8 Examples of Markov Processes . . . 66
3.8.1 The Wiener Process . . . 66
3.8.2 The Random Walk in One Dimension . . . 70
3.8.3 Poisson Process . . . 73
3.8.4 The Ornstein-Uhlenbeck Process . . . 74
3.8.5 Random Telegraph Process . . . 77

**4. The Ito Calculus and Stochastic Differential Equations** . . . 80
4.1 Motivation . . . 80
4.2 Stochastic Integration . . . 83
4.2.1 Definition of the Stochastic Integral . . . 83
4.2.2 Example $\int W(t')dW(t')$ . . . 84

4.2.3 The Stratonovich Integral . . . 86
4.2.4 Nonanticipating Functions . . . 86
4.2.5 Proof that $dW(tf = dt$ and $dW(t)^{2+N} = O$ . . . 87
4.2.6 Properties of the Ito Stochastic Integral . . . 88
4.3 Stochastic Differential Equations (SDE) . . . 92
4.3.1 Ito Stochastic Differential Equation: Definition . . . 93
4.3.2 Markov Property of the Solution of an Ito Stochastic Differential Equation . . . 95
4.3.3 Change of Variables: Ito's Formula . . . 95
4.3.4 Connection Between Fokker-Planck Equation and Stochastic Differential Equation . . . 96
4.3.5 Multivariable Systems . . . 97
4.3.6 Stratonovich's Stochastic Differential Equation . . . 98
4.3.7 Dependence on Initial Conditions and Parameters . . . 101
4.4 Some Examples and Solutions . . . 102
4.4.1 Coefficients Without $x$ Dependence . . . 102
4.4.2 Multiplicative Linear White Noise Process . . . 103
4.4.3 Complex Oscillator with Noisy Frequency . . . 104
4.4.4 Ornstein-Uhlenbeck Process . . . 106
4.4.5 Conversion from Cartesian to Polar Coordinates . . . 107
4.4.6 Multivariate Ornstein-Uhlenbeck Process . . . 109
4.4.7 The General Single Variable Linear Equation . . . 112
4.4.8 Multivariable Linear Equations . . . 114
4.4.9 Time-Dependent Ornstein-Uhlenbeck Process . . . 115

**5. The Fokker-Planck Equation** . . . 117
5.1 Background . . . 117
5.2 Fokker-Planck Equation in One Dimension . . . 118
5.2.1 Boundary Conditions . . . 118
5.2.2 Stationary Solutions for Homogeneous Fokker-Planck Equations . . . 124
5.2.3 Examples of Stationary Solutions . . . 126
5.2.4 Boundary Conditions for the Backward Fokker-Planck Equation . . . 128
5.2.5 Eigenfunction Methods (Homogeneous Processes) . . . 129
5.2.6 Examples . . . 132
5.2.7 First Passage Times for Homogeneous Processes . . . 136
5.2.8 Probability of Exit Through a Particular End of the Interval 142
5.3 Fokker-Planck Equations in Several Dimensions . . . 143
5.3.1 Change of Variables . . . 144
5.3.2 Boundary Conditions . . . 146
5.3.3 Stationary Solutions: Potential Conditions . . . 146
5.3.4 Detailed Balance . . . 148
5.3.5 Consequences of Detailed Balance . . . 150
5.3.6 Examples of Detailed Balance in Fokker-Planck Equations 155

5.3.7 Eigenfunction Methods in Many Variables—Homogeneous Processes . . . 165
5.4 First Exit Time from a Region (Homogeneous Processes) . . . 170
5.4.1 Solutions of Mean Exit Time Problems . . . 171
5.4.2 Distribution of Exit Points . . . 174

**6. Approximation Methods for Diffusion Processes . . . 177**
6.1 Small Noise Perturbation Theories . . . 177
6.2 Small Noise Expansions for Stochastic Differential Equations . . . 180
6.2.1 Validity of the Expansion . . . 182
6.2.2 Stationary Solutions (Homogeneous Processes) . . . 183
6.2.3 Mean, Variance, and Time Correlation Function . . . 184
6.2.4 Failure of Small Noise Perturbation Theories . . . 185
63 Small Noise Expansion of the Fokker-Planck Equation . . . 187
6.3.1 Equations for Moments and Autocorrelation Functions . . . 189
6.3.2 Example . . . 192
6.3.3 Asymptotic Method for Stationary Distributions . . . 194
6.4 Adiabatic Elimination of Fast Variables . . . 195
6.4.1 Abstract Formulation in Terms of Operators and Projectors . . . 198
6.4.2 Solution Using Laplace Transform . . . 200
6.4.3 Short-Time Behaviour . . . 203
6.4.4 Boundary Conditions . . . 205
6.4.5 Systematic Perturbative Analysis . . . 206
6.5 White Noise Process as a Limit of Nonwhite Process . . . 210
6.5.1 Generality of the Result . . . 215
6.5.2 More General Fluctuation Equations . . . 215
6.5.3 Time Nonhomogencous Systems . . . 216
6.5.4 Effect of Time Dependence in $L_1$ . . . 217
6.6 Adiabatic Elimination of Fast Variables: The General Case . . . 218
6.6.1 Example: Elimination of Short-Lived Chemical Intermediates . . . 218
6.6.2 Adiabatic Elimination in Haken's Model . . . 223
6.6.3 Adiabatic Elimination of Fast Variables: A Nonlinear Case . . . 227
6.6.4 An Example with Arbitrary Nonlinear Coupling . . . 232

**7. Master Equations and Jump Processes . . . 235**
7.1 Birth-Death Master Equations—One Variable . . . 236
7.1.1 Stationary Solutions . . . 236
7.1.2 Example: Chemical Reaction $X \rightleftarrows A$ . . . 238
7.1.3 A Chemical Bistable System . . . 241
7.2 Approximation of Master Equations by Fokker-Planck Equations . . . 246
7.2.1 Jump Process Approximation of a Diffusion Process . . . 246
7.2.2 The Kramers-Moyal Expansion . . . 245
7.2.3 Van Kampen's System Size Expansion . . . 250

7.2.4 Kurtz's Theorem . . . 254
7.2.5 Critical Fluctuations . . . 255
7.3 Boundary Conditions for Birth-Death Processes . . . 257
7.4 Mean First Passage Times . . . 259
7.4.1 Probability of Absorption . . . 261
7.4.2 Comparison with Fokker-Planck Equation . . . 261
7.5 Birth-Death Systems with Many Variables . . . 262
7.5.1 Stationary Solutions when Detailed Balance Holds . . . 263
7.5.2 Stationary Solutions Without Detailed Balance (Kirchoffs Solution) . . . 266
7.5.3 System Size Expansion and Related Expansions . . . 266
7.6 Some Examples . . . 267
7.6.1 $X + A \pm 2X$ . . . 267
7.6.2 $X \pm Y \rightleftarrows A$ . . . 267
7.6.3 Prey-Predator System . . . 268
7.6.4 Generating Function Equations . . . 273
7.7 The Poisson Representation . . . 277
7.7.1 Kinds of Poisson Representations . . . 282
7.7.2 Real Poisson Representations . . . 282
7.7.3 Complex Poisson Representations . . . 282
7.7.4 The Positive Poisson Representation . . . 285
7.7.5 Time Correlation Functions . . . 289
7.7.6 Trimolecular Reaction . . . 294
7.7.7 Third-Order Noise . . . 299

**8. Spatially Distributed Systems** . . . 303
8.1 Background . . . 303
8.1.1 Functional Fokker-Planck Equations . . . 305
8.2 Multivariate Master Equation Description . . . 307
8.2.1 Diffusion . . . 307
8.2.2 Continuum Form of Diffusion Master Equation . . . 308
8.2.3 Reactions and Diffusion Combined . . . 313
8.2.4 Poisson Representation Methods . . . 314
8.3 Spatial and Temporal Correlation Structures . . . 315
8.3.1 Reaction $X \rightleftarrows Y$ . . . 315
8.3.2 Reactions $B + X \rightleftarrows C, A + X \rightleftarrows 2X$ . . . 319
8.3.3 A Nonlinear Model with a Second-Order Phase Transition . . . 324
8.4 Connection Between Local and Global Descriptions . . . 328
8.4.1 Explicit Adiabatic Elimination of Inhomogeneous Modes . . . 328
8.5 Phase-Space Master Equation . . . 331
8.5.1 Treatment of Flow . . . 331
8.5.2 Flow as a Birth-Death Process . . . 332
8.5.3 Inclusion of Collisions—the Boltzmann Master Equation . . . 336
8.5.4 Collisions and Flow Together . . . 339

**9. Bistability, Metastability, and Escape Problems** . . . 342
9.1 Diffusion in a Double-Well Potential (One Variable) . . . 342
9.1.1 Behaviour for D = 0 . . . 343
9.1.2 Behaviour if /) is Very Small . . . 343
9.1.3 Exit Time . . . 345
9.1.4 Splitting Probability . . . 345
9.1.5 Decay from an Unstable State . . . 347
9.2 Equilibration of Populations in Each Well . . . 348
9.2.1 Kramers' Method . . . 349
9.2.2 Example: Reversible Denaturation of Chymotrypsinogen . 352
9.2.3 Bistability with Birth-Death Master Equations (One Variable) . . . 354
9.3 Bistability in Multivariable Systems . . . 357
9.3.1 Distribution of Exit Points . . . 357
9.3.2 Asymptotic Analysis of Mean Exit Time . . . 362
9.3.3 Kramers'Method in Several Dimensions . . . 363
9.3.4 Example: Brownian Motion in a Double Potential . . . 372

**10. Simulation of Stochastic Differential Equations** . . . 373
10.1 The One Variable Taylor Expansion . . . 374
10.1.1 Euier Methods . . . 374
10.1.2 Higher Orders . . . 374
10.1.3 Multiple Stochastic Integrals . . . 375
10.1.4 The Euler Algorithm . . . 375
10.1.5 Milstein Algorithm . . . 378
10.2 The Meaning of Weak and Strong Convergence . . . 379
10.3 Stability . . . 379
10.3.1 Consistency . . . 381
10.4 Implicit and Semi-implicit Algorithms . . . 382
10.5 Vector Stochastic Differential Equations . . . 383
10.5.1 Formulae and Notation . . . 383
10.5.2 Multiple Stochastic Integrals . . . 384
10.5.3 The Vector Euler Algorithm . . . 386
10.5.4 The Vector Milstein Algorithm . . . 386
10.5.5 The Strong Vector Semi-implicit Algorithm . . . 387
10.5.6 The Weak Vector Semi-implicit Algorithm . . . 387
10.6 Higher Order Algorithms . . . 388
10.7 Stochastic Partial Differential Equations . . . 389
10.7.1 Fourier Transform Methods . . . 390
10.7.2 The Interaction Picture Method . . . 390
10.8 Software Resources . . . 391

**References** . . . 393

**Bibliography** . . . 399

**Symbol Index** . . . . . **403**

**Author Index** . . . . . **407**

**Subject Index** . . . . . **409**