## Contents

	Preface Acknowledgements	page 1x xii
	Part I Introduction	1
1	Correlated Models and Wave Functions	3
	1.1 Introduction	3
	1.2 The Matrix Formulation	6
	1.3 Effective Lattice Models	7
	1.4 The Variational Principle	13
	1.5 Variational Wave Functions	14
	1.6 Size Extensivity	31
	1.7 Projection Techniques	34
	Part II Probability and Sampling	37
2	Probability Theory	39
	2.1 Introduction	39
	2.2 Events and Probability	41
	2.3 Moments of the Distribution: Mean Value and Variance	44
	2.4 Changing Random Variables	47
	2.5 The Chebyshev's Inequality	48
	2.6 Summing Independent Random Variables	48
	2.7 The Central Limit Theorem	53
3	Monte Carlo Sampling and Markov Chains	56
	3.1 Introduction	56
	3.2 Reweighting Technique and Correlated Sampling	59
	3.3 Direct Sampling	60
	3.4 Importance Sampling	61

vi Contents

	3.5	Sampling a Discrete Distribution Probability	62
	3.6	Sampling a Continuous Density Probability	64
	3.7	Markov Chains	66
	3.8	Detailed Balance and Approach to Equilibrium	69
	3.9	Metropolis Algorithm	74
	3.10	How to Estimate Errorbars	76
	3.11	Errorbars in Correlated Samplings	82
4	Lang	gevin Molecular Dynamics	85
	4.1	Introduction	85
	4.2	Discrete-Time Langevin Dynamics	87
	4.3	From the Langevin to the Fokker-Planck Equation	89
	4.4	Fokker-Planck Equation and Quantum Mechanics	91
	4.5	Accelerated Langevin Dynamics	96
	Part	t III Variational Monte Carlo	101
5	Vari	ational Monte Carlo	103
	5.1	Quantum Averages and Statistical Samplings	103
	5.2	The Zero-Variance Property	105
	5.3	Jastrow and Jastrow-Slater Wave Functions	106
	5.4	The Choice of the Basis Sets	108
	5.5	Bosonic Systems	109
	5.6	Fermionic Systems with Determinants	112
	5.7	Fermionic Systems with Pfaffians	123
	5.8	Energy and Correlation Functions	129
	5.9	Practical Implementation	129
5	Opti	mization of Variational Wave Functions	131
	6.1	Introduction	131
	6.2	Reweighting Techniques for the Optimization of Wave Functions	132
	6.3	Energy Derivatives	134
	6.4	The Stochastic Reconfiguration	137
	6.5	Stochastic Reconfiguration as a Projection Technique	146
	6.6	The Linear Method	147
	6.7	Calculations of Derivatives in the Jastrow-Slater Case	152
7	Tim	e-Dependent Variational Monte Carlo	156
	7.1	Introduction	156
	7.2	Real-Time Evolution of the Variational Parameters	157
	7.3	An Example for the Quantum Quench in One Dimension	161

	Contents	
	Part IV Projection Techniques	165
8	Green's Function Monte Carlo	167
	8.1 Basic Notions and Formal Derivations	167
	8.2 Single Walker Technique	170
	8.3 Importance Sampling	173
	8.4 The Continuous-Time Limit	178
	8.5 Many Walkers Formulation	180
	8.6 Practical Implementation	188
9	Reptation Quantum Monte Carlo	189
	9.1 A Simple Path Integral Technique	189
	9.2 A Simple Way to Sample Configurations	191
	9.3 The Bounce Algorithm	195
	9.4 The Continuous-Time Limit	196
	9.5 Practical Implementation	197
10	Fixed-Node Approximation	199
	10.1 The Sign Problem	199
	10.2 A Simple Example on the Continuum	204
	10.3 A Simple Example on the Lattice	208
	10.4 The Fixed-Node Approximation on the Lattice	209
	10.5 Practical Implementation	213
11	Auxiliary Field Quantum Monte Carlo	214
	11.1 Introduction	214
	11.2 Trotter Approximation	216
	11.3 Hubbard-Stratonovich Transformation	217
	11.4 The Path-Integral Representation	219
	11.5 Sequential Updates	223
	11.6 Ground-State Energy and Correlation Functions	228
	11.7 Simple Cases without Sign Problem	228
	11.8 Practical Implementation	231
	Part V Advanced Topics	233
12	Realistic Simulations on the Continuum	235
	12.1 Introduction and Motivations	235
	12.2 Variational Wave Function with Localized Orbitals	237
	12.3 Size Consistency of the Variational Wave Functions	244

viii Contents

12.4 Optimis	zation of the Variational Wave Functions	245
12.5 Lattice-	-Regularized Diffusion Monte Carlo	252
12.6 An Improved Scheme for the Lattice Regularization		
Appendix	Pseudo-Random Numbers Generated by Computers	261
References		264
Index		272