

# Contents

<b>1. Introduction: Purpose and Scope of this Volume, and Some General Comments . . . . .</b>	<b>1</b>
<b>2. Theoretical Foundations of the Monte Carlo Method and Its Applications in Statistical Physics . . . . .</b>	<b>5</b>
2.1 Simple Sampling Versus Importance Sampling . . . . .	5
2.1.1 Models . . . . .	5
2.1.2 Simple Sampling . . . . .	6
2.1.3 Random Walks and Self-Avoiding Walks . . . . .	8
2.1.4 Thermal Averages by the Simple Sampling Method . .	13
2.1.5 Advantages and Limitations of Simple Sampling . .	14
2.1.6 Importance Sampling . . . . .	17
2.1.7 More About Models and Algorithms . . . . .	20
2.2 Organization of Monte Carlo Programs, and the Dynamic Interpretation of Monte Carlo Sampling . .	23
2.2.1 First Comments on the Simulation of the Ising Model . . . . .	23
2.2.2 Boundary Conditions . . . . .	26
2.2.3 The Dynamic Interpretation of the Importance Sampling Monte Carlo Method . . . . .	29
2.2.4 Statistical Errors and Time-Displaced Relaxation Functions . . . . .	33
2.3 Finite-Size Effects . . . . .	35
2.3.1 Finite-Size Effects at the Percolation Transition . .	35
2.3.2 Finite-Size Scaling for the Percolation Problem . .	39
2.3.3 Broken Symmetry and Finite-Size Effects at Thermal Phase Transitions . . . . .	42
2.3.4 The Order Parameter Probability Distribution and Its Use to Justify Finite-Size Scaling and Phenomenological Renormalization . . . . .	44
2.3.5 Finite-Size Behavior of Relaxation Times . . . . .	54
2.3.6 Finite-Size Scaling Without “Hyperscaling” . . . .	57
2.3.7 Finite-Size Scaling for First-Order Phase Transitions . . . . .	58

2.3.8 Finite-Size Behavior of Statistical Errors and the Problem of Self-Averaging . . . . .	65
2.4 Remarks on the Scope of the Theory Chapter . . . . .	68
<b>3. Guide to Practical Work with the Monte Carlo Method . . . . .</b>	<b>69</b>
3.1 Aims of the Guide . . . . .	72
3.2 Simple Sampling . . . . .	74
3.2.1 Random Walk . . . . .	74
3.2.2 Nonreversal Random Walk . . . . .	82
3.2.3 Self-Avoiding Random Walk . . . . .	83
3.2.4 Percolation . . . . .	87
3.3 Biased Sampling . . . . .	95
3.3.1 Self-Avoiding Random Walk . . . . .	95
3.4 Importance Sampling . . . . .	98
3.4.1 Ising Model . . . . .	98
3.4.2 Self-Avoiding Random Walk . . . . .	112
<b>4. Some Important Recent Developments of the Monte Carlo Methodology . . . . .</b>	<b>115</b>
4.1 Introduction . . . . .	115
4.2 Application of the Swendsen–Wang Cluster Algorithm to the Ising Model . . . . .	117
4.3 Reweighting Methods in the Study of Phase Diagrams, First-Order Phase Transitions, and Interfacial Tensions . . . . .	122
4.4 Some Comments on Advances with Finite-Size Scaling Analyses . . . . .	127
<b>5. Quantum Monte Carlo Simulations: An Introduction . . . . .</b>	<b>137</b>
5.1 Quantum Statistical Mechanics vs. Classical Statistical Mechanics . . . . .	137
5.2 The Path Integral Quantum Monte Carlo Method (PIMC) . .	143
5.3 Quantum Monte Carlo for Lattice Models . . . . .	150
5.4 Concluding Remarks . . . . .	158
<b>Appendix . . . . .</b>	<b>159</b>
A.1 Algorithm for the Random Walk Problem . . . . .	159
A.2 Algorithm for Cluster Identification . . . . .	160
<b>References . . . . .</b>	<b>165</b>
<b>Bibliography . . . . .</b>	<b>175</b>
<b>Subject Index . . . . .</b>	<b>177</b>