

Contents

1	Introduction: Purpose and Scope of This Volume, and Some General Comments	1
2	Theoretical Foundations of the Monte Carlo Method and Its Applications in Statistical Physics	5
2.1	Simple Sampling Versus Importance Sampling	5
2.1.1	Models	5
2.1.2	Simple Sampling	7
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	25
2.2.3	The Dynamic Interpretation of the Importance Sampling Monte Carlo Method	28
2.2.4	Statistical Errors and Time-Displaced Relaxation Functions	32
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	38
2.3.3	Broken Symmetry and Finite-Size Effects at Thermal Phase Transitions	41
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	52
2.3.6	Finite-Size Scaling Without “Hyperscaling”	56
2.3.7	Finite-Size Scaling for First-Order Phase Transitions	56
2.3.8	Finite-Size Behavior of Statistical Errors and the Problem of Self-Averaging	62
2.4	Remarks on the Scope of the Theory Chapter	67

3	Guide to Practical Work with the Monte Carlo Method	69
3.1	Aims of the Guide	71
3.2	Simple Sampling	74
3.2.1	Random Walk	74
3.2.2	Nonreversal Random Walk	81
3.2.3	Self-Avoiding Random Walk	82
3.2.4	Percolation	86
3.3	Biased Sampling	93
3.3.1	Self-Avoiding Random Walk	94
3.4	Importance Sampling	96
3.4.1	Ising Model	96
3.4.2	Self-Avoiding Random Walk	110
4	Some Important Recent Developments of the Monte Carlo Methodology	111
4.1	Introduction	111
4.2	Application of the Swendsen–Wang Cluster Algorithm to the Ising Model	113
4.3	Reweighting Methods in the Study of Phase Diagrams, First-Order Phase Transitions, and Interfacial Tensions	118
4.4	Some Comments on Advances with Finite-Size Scaling Analyses	123
5	Quantum Monte Carlo Simulations: An Introduction	131
5.1	Quantum Statistical Mechanics Versus Classical Statistical Mechanics	131
5.2	The Path Integral Quantum Monte Carlo Method	137
5.3	Quantum Monte Carlo for Lattice Models	143
5.4	Concluding Remarks	152
6	Monte Carlo Methods for the Sampling of Free Energy Landscapes	153
6.1	Introduction and Overview	153
6.2	Umbrella Sampling	161
6.3	Multicanonical Sampling and Other “Extended Ensemble” Methods	164
6.4	Wang–Landau Sampling	166
6.5	Transition Path Sampling	169
6.6	Concluding Remarks	173
	Appendix	175
A.1	Algorithm for the Random Walk Problem	175
A.2	Algorithm for Cluster Identification	176
	References	181
	Bibliography	193
	Subject Index	197