Kurt Binder Dieter W. Heermann

## Monte Carlo Simulation in Statistical Physics

An Introduction

Fifth Edition

With 54 Figures



## **Contents**

1	Intro	Introduction: Purpose and Scope of This Volume, and Some					
	Gen	eral Co	mments	1			
2	The	oretical	Foundations of the Monte Carlo Method				
			lications in Statistical Physics	5			
	2.1		e Sampling Versus Importance Sampling				
		2.1.1	Models				
		2.1.2	Simple Sampling				
		2.1.3	Random Walks and Self-Avoiding Walks				
		2.1.4	Thermal Averages by the Simple Sampling Method				
		2.1.5	Advantages and Limitations of Simple Sampling				
		2.1.6	Importance Sampling				
		2.1.7	More About Models and Algorithms	20			
	2.2	Organ	ization of Monte Carlo Programs, and the Dynamic				
		Interp	retation 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				
		2.2.4	Statistical Errors and Time-Displaced Relaxation Functions	32			
	2.3	Finite-	-Size Effects				
		2.3.1	Finite-Size Effects at the Percolation Transition				
		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				
		2.3.5	Finite-Size Behavior of Relaxation Times				
		2.3.6	Finite-Size Scaling Without "Hyperscaling"				
		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				
	2.4	Remai	rks on the Scope of the Theory Chapter	67			

3	Guide to Practical Work with the Monte Carlo Method					
	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				
	3.3	Biased Sampling				
		3.3.1 Self-Avoiding Random Walk				
	3.4	Importance Sampling				
		3.4.1 Ising Model				
		3.4.2 Self-Avoiding Random Walk				
4	Som	e Important Recent Developments of the Monte Carlo				
	Met	hodology	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					
	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				
	5.4	Concluding Remarks				
6	Monte Carlo Methods for the Sampling of Free Energy Landscapes					
	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			
ΑĮ	pend	ix				
_	A.1	Algorithm for the Random Walk Problem	175			
	A.2	Algorithm for Cluster Identification	176			
Re	eferen	ices	181			
Bi	bliogi	raphy	193			
DÜ	wject	Index	197			