

Contents

1. <i>Introduction: Theory and "Technical" Aspects of Monte Carlo Simulations</i>	
By K. Binder (With 5 Figures)	1
1.1 Purpose of the Monte Carlo Method	1
1.2 Description of the Monte Carlo Technique in Classical Statistical Mechanics	3
1.2.1 Computation of Static Averages in the Canonic Ensemble	3
1.2.2 Estimation of the Free Energy. Practical Realization. Other Ensembles	7
1.2.3 Dynamic Interpretation of the Monte Carlo Process	12
1.2.4 Accuracy Considerations: Pseudorandom Numbers, Finite Time Averaging, Initial Condition, etc.	16
1.2.5 Appropriate Choice of Boundary Conditions	22
1.2.6 Finite Size Problems. The Extrapolation to the Thermodynamic Limit	26
1.3 Aspects of Simulations of Kinetic Processes	30
1.3.1 Various Monte Carlo Realizations of the Same Master Equation ..	30
1.3.2 Computations with Conservation Laws: "Hydrodynamic" Slowing Down	34
1.3.3 Slowing Down at Phase Transitions. How to Estimate the Order of a Transition	36
1.4 Variants of the Monte Carlo Method	38
1.4.1 The Approximation of Alexandrowicz	38
1.4.2 Renormalization Group Treatments Utilizing Monte Carlo Methods	40
1.5 Conclusions	41
References	43
Addendum	45
2. <i>Simulation of Classical Fluids.</i>	
By D. Levesque, J.-J. Weis, and J.-P. Hansen	47
2.1 Overview	47
2.2 Hard Core and Discontinuous Potentials	49
2.2.1 Hard-Sphere System	49

a)	The Pure Hard-Sphere System	49
The Equation of State		49
The Correlation Functions of the Hard-Sphere System		54
b)	Hard-Sphere Mixture	57
Mixtures of Hard Spheres with Additive Diameter		58
Mixtures of Hard Spheres with Nonadditive Diameter		59
2.2.2	Hard Spheres with Discontinuous Short-Range Potential	60
a)	Hard Spheres with a Square Well	60
b)	Hard Spheres with a Triangular Well	61
c)	The Hard Spheres with a Repulsive Square Well	61
d)	Mixtures of Hard Spheres and Hard Spheres Plus Square Well	61
e)	Conclusion	62
2.2.3	Two-Dimensional Systems	62
a)	The Hard-Disk System	62
b)	The Mixtures of Hard Disks	64
c)	System with a Repulsive "Step" Potential	65
d)	The Hard Parallel Square System	65
2.3	Soft Short-Range Potentials	66
2.3.1	Inverse Power Potentials	66
a)	The Inverse-12 Potential	66
b)	The Inverse-9, -6 and -4 Potentials	67
2.3.2	The Lennard-Jones (LJ) Potential	68
a)	The Pure Lennard-Jones (LJ) System	68
The Thermodynamic Properties		68
The Correlation Functions		71
b)	Conclusion	71
c)	The Lennard-Jones (LJ) Mixtures	72
2.3.3	The Two-Dimensional Lennard-Jones (LJ) System	73
2.4	Ionic Systems	74
2.4.1	Generalities	74
a)	Specific Problems	74
b)	Classes of Ionic Fluids	77
2.4.2	Fully Ionized Matter	77
a)	The One Component Plasma	78
b)	Electron Screening	80
c)	Charged Hard Spheres in a Uniform Background	80
d)	Ionic Mixtures	81
e)	Hydrogen Plasmas	82
2.4.3	The Primitive Model and Its Applications	83
a)	The Restricted Primitive Model	83
b)	The Dissymmetric Primitive Model	87

2.4.4	Molten Salts	87
a)	Potentials	87
b)	KCl	88
c)	Other Alkali Halides	90
d)	Corresponding States Model	91
e)	Mixtures	91
2.4.5	Liquid Metals	91
a)	Generalities	91
b)	"Realistic" Potentials	92
2.5	Molecular Fluids	93
2.5.1	Hard Convex Bodies	95
a)	Hard Spherocylinders (3-dim.)	95
b)	Hard Ellipsoids (3-dim.)	96
c)	Hard Ellipses (2-dim.)	97
d)	Hard Spherocylinders (2-dim.)	97
2.5.2	Atom-Atom Potentials	98
a)	Hard Diatomics (Fused Hard-Spheres, Dumbbells)	98
b)	Lennard-Jones Atom-Atom Potentials	102
c)	Other Atom-Atom Potentials	104
2.5.3	Generalized Stockmayer Potentials	104
a)	Dipole-Dipole Interaction	105
b)	Quadrupole-Quadrupole Interaction	111
c)	Dipole-Quadrupole Interaction	111
d)	Anisotropic Overlap Interaction	111
2.6	Gas-Liquid Interface	112
	References	114

3. *Phase Diagrams of Mixtures and Magnetic Systems*

By D.P. Landau (With 13 Figures)	121
3.1 Ordinary Phase Transitions in Magnets and Binary Alloys	121
3.1.1 Ising Model	122
3.1.2 Magnetic Systems with Isotropic Interactions	128
3.2 Multicritical Points and Crossover Behavior	132
3.2.1 Tricritical Phenomena	133
3.2.2 Bicritical and Other Multicritical Behavior	135
3.3 Phase Transitions in Miscellaneous Systems	139
3.4 Conclusions	141
References	141
Addendum	144

4. *Quantum Many-Body Problems*

By D.M. Ceperley and M.H. Kalos (With 4 Figures)	145
Abstract	145
4.1 Introductory Remarks	146
4.2 Variational Methods	146
4.2.1 Monte Carlo Methods with the Product Trial Function	149
a) Finite System Size	150
b) The Random Walk	151
c) Computation of the Pseudopotential	151
d) Fermion Trial Function	152
e) Computing the Trial Energy	153
f) The Pressure	154
g) The Single Particle Density Matrix	155
h) Reweighting Configurations	155
4.2.2 Application to Systems of Helium	156
a) Hard-Core Boson Systems	157
b) Liquid ^4He	157
c) Solid ^4He and ^3He	160
d) Interatomic Helium Potential	161
e) The Hard-Sphere Potential	161
f) Nonuniform Helium Systems	162
g) Two-Dimensional Helium	163
h) Three-Body Pseudopotential	164
4.2.3 Other Bose Systems	164
a) Spin-Aligned Hydrogen	164
b) Soft-Core Bose Systems	166
c) Bose Neutron Matter Calculations	166
d) Bose One-Component Plasma	167
4.2.4 Fermi Liquids	169
a) Helium Three	171
b) Neutron Matter	171
c) Yukawa Fermions	172
d) The Electron Gas	172
4.2.5 Monte Carlo Techniques for Low-Temperature Excitations	173
4.3 Nearly Classical Systems	174
4.4 The Green's Function Monte Carlo Method (GFMC)	175
a) Schrödinger's Equation in Integral Form	175
b) Sampling Green's Function by Random Walks	179
c) Importance Sampling	181
d) Quantum Mechanical Expectations	183
e) Implementation	185

4.4.1 Results	186
4.5 Virial Coefficients and Pair Correlations	190
4.6 Conclusions	191
References	192
5. <i>Simulation of Small Systems</i> . By H. Müller-Krumbhaar (With 9 Figures)	195
5.1 Introductory Remarks	195
5.2 Statics	197
5.2.1 Clusters in Continuous Space	197
5.2.2 Lattice Models	199
a) General Remarks	199
b) Finite-Size Behavior and Superparamagnetism	200
c) Equilibrium Cluster Statistics in Systems with Interaction	204
d) Cluster Statistics in the Percolation Problem	210
5.3 Cluster Dynamics	213
5.3.1 First-Order Phase Transitions	213
5.3.2 Second-Order Transitions	216
Appendix	219
Cluster Counting Algorithm	219
References	221
Addendum	223
6. <i>Monte Carlo Studies of Relaxation Phenomena: Kinetics of Phase Changes and Critical Slowing Down</i> . By K. Binder and M.H. Kalos (With 15 Figures)	225
6.1 Introductory Remarks	225
6.2 Kinetics of Fluctuations in Thermal Equilibrium	228
6.2.1 Dynamics of Models for Chain Molecules	228
6.2.2 Critical Slowing Down in Systems Without Conservation Laws ..	230
6.2.3 Relaxation in Systems with Conserved Quantities	232
6.2.4 Dynamics at a Multicritical Point	234
6.2.5 Dynamics of "Clusters": Their Reaction Rate and Diffusion Constant	235
6.3 Kinetics of Nonlinear Relaxation	238
6.3.1 Nonlinear Critical Slowing Down	238
6.3.2 Nucleation Kinetics at First-Order Phase Transitions	239
6.3.3 Kinetics of Spinodal Decomposition and Grain Growth in Alloys	248
6.4 Conclusions and Outlook	253
References	258

7. <i>Monte Carlo Simulation of Crystal Growth</i>	
By H. Müller-Krumbhaar (With 17 Figures)	261
7.1 Introductory Remarks	261
7.2 Crystal Surfaces at Equilibrium	263
7.2.1 Singular Faces	263
a) Kossel Model (Simple Cubic-(100) Face), Two-Dimensional Spin-s-Ising Model, Thin Films	263
b) Other Low-Index Faces	267
7.2.2 Surface Steps	268
7.2.3 Roughening Transition	269
7.3 Growth Kinetics	272
7.3.1 General Aspects of Kinetic Simulations in Crystal Growth	272
7.3.2 Low-Index Faces	274
a) Two-Dimensional Ising Model	274
b) Kossel Model (100) Face	276
c) Orientational Dependence of the Growth Rate (sc-, fcc-Lattices)	278
d) Adsorption on a Substrate	280
e) Surface Diffusion	281
7.3.3 Surface Steps	282
a) Straight Steps	282
b) Spiral Growth and Spreading of Two-Dimensional Nuclei	283
7.3.4 Roughening Transition	288
7.3.5 More Component Crystals and Segregation of Impurities	290
7.4 Outlook	293
References	296
8. <i>Monte Carlo Studies of Systems with Disorder</i>	
By K. Binder and D. Stauffer (With 17 Figures)	301
8.1 Dilute Impurities in Magnets	302
8.2 Dilute Ferromagnets and the Percolation Problem	304
8.2.1 Thermodynamic Properties at Nonzero Temperatures	304
8.2.2 Percolation Cluster Numbers at Zero Temperatures	305
8.2.3 Cluster Surfaces and Correlations	312
8.2.4 Conductivity and Spin Waves	314
8.2.5 Miscellaneous Topics	316
8.3 Spin Glasses	317
8.3.1 Physical Properties of Spin Glass Systems	317
8.3.2 Distribution of Interactions and Effective Fields	319
8.3.3 Susceptibility and Specific Heat	319
8.3.4 Magnetization and Order Parameters	321

8.3.5	Kinetic Phenomena	325
8.3.6	Ground-State Properties	325
8.4	Disordered Heteropolymers and Their Helix-Coil Transition	326
8.5	Structurally Disordered Solids (Glasses etc.)	328
8.6	Conclusions and Outlook	330
	References	333
9.	<i>Applications in Surface Physics</i> . By D.P. Landau (With 11 Figures)	337
9.1	Introductory Remarks	337
9.2	Critical Behavior of Magnetic Systems with Surfaces	338
9.3	Surface Effects in Binary Alloys	343
9.3.1	Surface Enrichment	343
9.3.2	Surface Critical Phenomena	345
9.4	Phase Transitions in Adsorbed Surface Layers	347
9.4.1	Lattice Gas Models	347
9.4.2	"Continuum" Models	352
9.5	Kinetic Phenomena at Surfaces	352
9.6	Conclusions	353
	References	354
	Addendum	355
10.	<i>Recent Trends in the Development and Application of the Monte Carlo Method</i> . By K. Binder (With 6 Figures)	357
10.1	Performance of Monte Carlo Programs	358
10.1.1	General Comments	358
10.1.2	Monte Carlo Calculations on Special-Purpose Computers ...	359
10.1.3	Speeding-up of Monte Carlo Programs on Vector Processors .	361
10.2	Some Comments on Finite-Size Effects	364
10.2.1	Statement of the Problem	364
10.2.2	Standard Finite-Size Scaling Theory	365
10.2.3	Phenomenological Renormalization of Monte Carlo Data	367
10.2.4	Finite-Size Effects at First-Order Phase Transitions	372
10.3	New Directions for the Application of the Monte Carlo Method	374
10.3.1	Monte Carlo Renormalization Group (MCRG)	374
10.3.2	Applications to Lattice Gauge Theory	377
10.3.3	Kinetics of Aggregation and Growth Phenomena	380
10.4	Quantum Statistical Mechanics on Lattices	382
10.5	Concluding Remarks	386
	References	388
	Addendum	393
	Subject Index	399