Table of Contents

1. Introduction 1

2. Computer Methods in the Study of Phase Transitions and Critical Phenomena 3
2.1 Statistical Mechanics and Phase Transitions 5
2.1.1 Modern theories of phase transitions and critical phenomena 5
2.1.2 Statistical mechanics, order parameters, fluctuations, critical exponents, scaling, and universality 6
2.2 Numerical Simulation Techniques 9
2.2.1 Monte Carlo methods 9
2.2.2 A Monte Carlo importance-sampling method 10
2.2.3 A realization of a Monte Carlo method 13
2.2.4 General limitations of the Monte Carlo method 15
2.2.5 Broken ergodicity 15
2.2.6 Distribution functions 18
2.2.7 Coarse-graining techniques and criteria of convergence 19
2.2.8 Finite-size effects 20
2.2.9 Determining the nature of a phase transition 22
2.2.10 Computational details 27
2.2.11 General advantages of the Monte Carlo method: Applications 28
2.3 Exact Configurational Counting and Series Expansions 29
2.3.1 A general approach 29
2.3.2 The moment method 31
2.3.3 Principles of the calculation 32
2.3.4 Step 1. Determination of all distinct graphs and their multiplicities 33
2.3.5 Step 2. Embedding of connected graphs into a lattice . . 35
2.3.6 General correlation function series 36
2.3.7 Capabilities and limitations of a general approach . . . 37

3. Monte Carlo Pure-model Calculations 39
3.1 Critical Behavior of the Three-dimensional Ising Model . . . 40
3.1.1 The Ising model and its order parameter 40

3.1.2 Numerical evidence of a phase transition in the Ising model on a diamond lattice 41
3.1.3 Finite-size scaling analysis and critical behavior 43
3.1.4 Are Monte Carlo techniques practicable in the study of critical phenomena? 47
3.2 Phase Behavior of Ising Models with Multi-spin Interactions 48
3.2.1 Higher-order exchange in magnetic systems 48
3.2.2 Ising models with multi-spin interactions 48
3.2.3 First-order phase transitions of Ising models with pure multi-spin interactions 49
3.2.4 Universality and tricritical behavior of Ising models with two- and four-spin interactions: Pair interactions as a symmetry-breaking field 57
3.3 Thermodynamics of One-dimensional Heisenberg Models . . 67
3.3.1 One-dimensional magnetic models 67
3.3.2 The anisotropic Heisenberg model in a magnetic field 69
3.3.3 Comparison with theoretical calculations on a continuum model 72
3.3.4 A model of the linear magnet $CsNiF_3$? 74

4. Testing Modern Theories of Critical Phenomena 77
4.1 Fluctuation-induced First-order Phase Transitions 78
4.1.1 The role of fixed points in the renormalization group theory 78
4.1.2 Motivation for computer studies of fluctuation-induced first-order phase transitions 79
4.1.3 Phase transitions in antiferromagnets with order parameters of dimension $n=6$ and $n=3$ 80
4.1.4 Crossover from first-order to continuous transitions in a symmetry-breaking field 85
4.1.5 Fluctuation-induced first-order phase transitions in Ising models with competing interactions 90
4.2 Critical Phenomena at Marginal Dimensionality 93
4.2.1 The role of a marginal spatial dimension 93
4.2.2 Computer experiments of hypercubic Ising models: »A romance of many dimensions« 95
4.2.3 Susceptibility and critical isotherm of the four-dimensional Ising model 99
4.2.4 Conclusions on critical behavior in marginal dimensions 100
4.3 Basic Assumptions of Critical Correlation Theories 101
4.3.1 Review of a critical correlation theory 101
4.3.2 Testing the basic assumption by Monte Carlo calculations 103

5. Numerical Experiments 107
5.1 Phase Transitions in Lipid Bilayers and Biological Membranes 108
5.1.1 What are biological membranes and what do they do? . 108
5.1.2 Lipid bilayers are model membranes 109
5.1.3 Phase behavior of lipid bilayers 110
5.1.4 Back to biology: Are phase transitions at all relevant to the biological functions of the membrane? 110
5.1.5 Theories of lipid bilayer phase transitions 111
5.1.6 Computer simulations of lipid bilayers 112
5.1.7 Multi-state models of lipid bilayers 113
5.1.8 Computer simulations of the q-state models for the gel-fluid phase transition 116
5.1.9 Computer simulation of the phase behavior of lipid bilayers with »impurities«: cholesterol, proteins, and polypeptides 124
5.1.10 Have computer studies provided any new insight into the properties of biological membranes? 127
5.2 Nuclear Dipolar Magnetic Ordering and Phase Transitions . . 128
5.2.1 Nuclear dipolar magnetic ordering 128
5.2.2 The secular dipolar Hamiltonian 129
5.2.3 Perspectives in studies of nuclear dipolar magnetic ordering 130
5.2.4 Motivation for a numerical simulation study of nuclear dipolar magnetic ordering 131
5.2.5 Monte Carlo studies of systems with truncated classical secular dipolar interactions 132
5.2.6 Nature of the spin structures: »Permanent« structures or the devil's staircase? 133
5.2.7 Double-layered spin structures in CaF_2-like systems: Continuous transitions and critical behavior 138
5.2.8 Multi-layered spin structures in CaF_2-like systems: Firstorder phase transitions 144
5.2.9 Can series expansions provide information on the nature of the phase transitions? 145
5.2.10 Nuclear antiferrimagnetic susceptibilities of systems with two spin species: LiF and LiH 146
5.3 Phase Transitions of Adsorbed Monolayers 148
5.3.1 Two-dimensional phases of molecules adsorbed on solid surfaces 148
5.3.2 N_2 physisorbed on graphite: The anisotropic-planar rotor model 149
5.3.3 The Heisenberg model with cubic anisotropy 152
5.3.4 Fluctuation-induced first-order phase transition in the anisotropic-planar rotor model 153

5.3.5 Comparison with experiments on N_2 physisorbed on graphite 160
5.3.6 Phase behavior on the anisotropic-planar rotor model with vacancies 162
5.3.7 Physical realizations of the anisotropic-planar rotor model with vacancies 170
5.4 Kinetics of Growth 170
5.4.1 Growth 170
5.4.2 Computer simulation of domain-growth kinetics 172
5.4.3 Domain-growth kinetics of herringbone phases 173
5.4.4 Domain-growth kinetics of pinwheel phases 181
5.4.5 Kinetics of growth and critical phenomena 182

Bibliography 185

Subject Index 197