

Contents

Part I Molecular Dynamics

1 Introduction to Molecular Dynamics

<i>Ralf Schneider, Amit Raj Sharma, and Abha Rai</i>	3
1.1 Basic Approach	3
1.2 Macroscopic Parameters	6
1.3 Inter-Atomic Potentials	8
1.4 Numerical Integration Techniques	14
1.5 Analysis of MD Runs	18
1.6 From Classical to Quantum-Mechanical MD	23
1.7 Ab Initio MD	24
1.8 Car-Parrinello Molecular Dynamics	25
1.9 Potential Energy Surface	28
1.10 Advanced Numerical Methods	29
References	37

2 Wigner Function Quantum Molecular Dynamics

<i>V. S. Filinov, M. Bonitz, A. Filinov, and V. O. Golubnychiy</i>	41
2.1 Quantum Distribution Functions	41
2.2 Semiclassical Molecular Dynamics	43
2.3 Quantum Dynamics	50
2.4 Time Correlation Functions in the Canonical Ensemble	54
2.5 Discussion	58
References	59

Part II Classical Monte Carlo

3 The Monte Carlo Method, an Introduction

<i>Detlev Reiter</i>	63
3.1 What is a Monte Carlo Calculation?	63
3.2 Random Number Generation	67
3.3 Integration by Monte Carlo	71
3.4 Summary	77
References	78

4 Monte Carlo Methods in Classical Statistical Physics

Wolfhard Janke 79

4.1 Introduction 79

4.2 Statistical Physics Primer 80

4.3 The Monte Carlo Method 85

4.4 Cluster Algorithms 93

4.5 Statistical Analysis of Monte Carlo Data 99

4.6 Reweighting Techniques 108

4.7 Finite-Size Scaling Analysis 114

4.8 Generalized Ensemble Methods 129

4.9 Concluding Remarks 135

References 135

5 The Monte Carlo Method for Particle Transport Problems

Detlev Reiter 141

5.1 Transport Problems and Stochastic Processes 141

5.2 The Transport Equation: Fredholm Integral
Equation of Second Kind 143

5.3 The Boltzmann Equation 144

5.4 The Linear Integral Equation for the Collision Density 147

5.5 Monte Carlo Solution 150

5.6 Some Special Sampling Techniques 154

5.7 An Illustrative Example 156

References 158

Part III Kinetic Modelling

6 The Particle-in-Cell Method

David Tskhakaya 161

6.1 General Remarks 161

6.2 Integration of Equations of Particle Motion 163

6.3 Plasma Source and Boundary Effects 166

6.4 Calculation of Plasma Parameters and Fields
Acting on Particles 170

6.5 Solution of Maxwell’s Equations 175

6.6 Particle Collisions 183

6.7 Final Remarks 188

References 188

**7 Gyrokinetic and Gyrofluid Theory and Simulation
of Magnetized Plasmas**

Richard D. Sydora 191

7.1 Introduction 191

7.2 Single Particle Dynamics 193

7.3 Continuum Gyrokinetics 200

7.4	Gyrofluid Model	204
7.5	Gyrokinetic Particle Simulation Model	207
7.6	Gyrokinetic Particle Simulation Model Applications	210
7.7	Summary	217
	References	218

Part IV Semiclassical Approaches

8 Boltzmann Transport in Condensed Matter

	<i>Franz Xaver Bronold</i>	223
8.1	Boltzmann Equation for Quasiparticles	223
8.2	Techniques for the Solution of the Boltzmann Equation	230
8.3	Conclusions	252
	References	253

9 Semiclassical Description of Quantum Many-Particle Dynamics in Strong Laser Fields

	<i>Thomas Fennel and Jörg Köhn</i>	255
9.1	Semiclassical Many-Particle Dynamics in Mean-Field Approximation	255
9.2	Semiclassical Ground State	261
9.3	Application to Simple-Metal Clusters	265
	References	272

Part V Quantum Monte Carlo

10 World-line and Determinantal Quantum Monte Carlo Methods for Spins, Phonons and Electrons

	<i>F.F. Assaad and H.G. Evertz</i>	277
10.1	Introduction	277
10.2	Discrete Imaginary Time World Lines for the XXZ Spin Chain	278
10.3	World-Line Representations without Discretization Error	299
10.4	Loop Operator Representation of the Heisenberg Model	303
10.5	Spin-Phonon Simulations	308
10.6	Auxiliary Field Quantum Monte Carlo Methods	312
10.7	Numerical Stabilization Schemes for Lattice Models	325
10.8	The Hirsch-Fye Impurity Algorithm	337
10.9	Selected Applications of the Auxiliary Field Method	344
10.10	Conclusion	345
10.A	The Trotter Decomposition	345

10.B	The Hubbard-Stratonovich Decomposition	347
10.C	Slater Determinants and their Properties	349
	References	353

11 Autocorrelations in Quantum Monte Carlo Simulations of Electron-Phonon Models

<i>Martin Hohenadler and Thomas C. Lang</i>	357	
11.1	Introduction	357
11.2	Holstein Model	358
11.3	Numerical Methods	358
11.4	Problem of Autocorrelations	360
11.5	Origin of Autocorrelations and Principal Components	363
11.6	Conclusions	365
	References	366

12 Diagrammatic Monte Carlo and Stochastic Optimization Methods for Complex Composite Objects in Macroscopic Baths

<i>A. S. Mishchenko</i>	367	
12.1	Introduction	367
12.2	Physical Properties of Interest	372
12.3	The Diagrammatic Monte Carlo Method	374
12.4	Stochastic Optimization Method	391
12.5	Conclusions and Perspectives	393
	References	394

13 Path Integral Monte Carlo Simulation of Charged Particles in Traps

<i>Alexei Filinov, Jens Böning, and Michael Bonitz</i>	397	
13.1	Introduction	397
13.2	Idea of Path Integral Monte Carlo	397
13.3	Basic Numerical Issues of PIMC	401
13.4	PIMC for Degenerate Bose Systems	406
13.5	Discussion	410
	References	411

Part VI Ab-Initio Methods in Physics and Chemistry

14 Ab-Initio Approach to the Many-Electron Problem

<i>Alexander Quandt</i>	415	
14.1	Introduction	415
14.2	An Orbital Approach to Chemistry	419
14.3	Hartree-Fock Theory	427
14.4	Density Functional Theory	432
	References	435

15 Ab-Initio Methods Applied to Structure Optimization and Microscopic Modelling

<i>Alexander Quandt</i>	437
15.1 Exploring Energy Hypersurfaces	437
15.2 Applied Theoretical Chemistry	444
15.3 Model Hamiltonians	451
15.4 Summary and Outlook	465
15.A Links to Popular Ab Initio Packages	466
References	467

Part VII Effective Field Approaches

16 Dynamical Mean-Field Approximation and Cluster Methods for Correlated Electron Systems

<i>Thomas Pruschke</i>	473
16.1 Introduction	473
16.2 Mean-Field Theory for Correlated Electron Systems	475
16.3 Extending the DMFT: Effective Cluster Theories	492
16.4 Conclusions	499
References	501

17 Local Distribution Approach

<i>Andreas Alvermann and Holger Fehske</i>	505
17.1 Introduction	505
17.2 Applications of the LD Approach	514
17.3 Summary	525
References	526

Part VIII Iterative Methods for Sparse Eigenvalue Problems

18 Exact Diagonalization Techniques

<i>Alexander Weiße and Holger Fehske</i>	529
18.1 Basis Construction	529
18.2 Eigenstates of Sparse Matrices	539
References	543

19 Chebyshev Expansion Techniques

<i>Alexander Weiße and Holger Fehske</i>	545
19.1 Chebyshev Expansion and Kernel Polynomial Approximation	545
19.2 Applications of the Kernel Polynomial Method	554
19.3 KPM in Relation to other Numerical Approaches	568
References	575

**Part IX The Density Matrix Renormalisation Group:
Concepts and Applications**

20 The Conceptual Background of Density-Matrix Renormalization

<i>Ingo Peschel and Viktor Eisler</i>	581
20.1 Introduction	581
20.2 Entangled States	581
20.3 Reduced Density Matrices	582
20.4 Solvable Models	583
20.5 Spectra	586
20.6 Entanglement Entropy	589
20.7 Matrix-Product States	593
20.8 Summary	594
References	594

21 Density-Matrix Renormalization Group Algorithms

<i>Eric Jeckelmann</i>	597
21.1 Introduction	597
21.2 Matrix-Product States and (Super-)Blocks	598
21.3 Numerical Renormalization Group	600
21.4 Infinite-System DMRG Algorithm	602
21.5 Finite-System DMRG Algorithm	607
21.6 Additive Quantum Numbers	611
21.7 Truncation Errors	613
21.8 Computational Cost and Optimization	616
21.9 Basic Extensions	617
References	618

22 Dynamical Density-Matrix Renormalization Group

<i>Eric Jeckelmann and Holger Benthien</i>	621
22.1 Introduction	621
22.2 Methods for Simple Discrete Spectra	623
22.3 Dynamical DMRG	626
22.4 Finite-Size Scaling	630
22.5 Momentum-Dependent Quantities	631
22.6 Application: Spectral Function of the Hubbard Model	632
References	634

**23 Studying Time-Dependent Quantum Phenomena
with the Density-Matrix Renormalization Group**

<i>Reinhard M. Noack, Salvatore R. Manmana, Stefan Wessel, and Alejandro Muramatsu</i>	637
23.1 Time Dependence in Interacting Quantum Systems	637
23.2 Sudden Quench of Interacting Fermions	643
23.3 Discussion	650
References	651

24 Applications of Quantum Information in the Density-Matrix Renormalization Group

Ö. Legeza, R.M. Noack, J. Sólyom, and L. Tincani 653

24.1 Basic Concepts of Quantum Information Theory 653

24.2 Entropic Analysis of Quantum Phase Transitions 657

24.3 Discussion and Outlook 662

References 663

25 Density-Matrix Renormalization Group for Transfer Matrices: Static and Dynamical Properties of 1D Quantum Systems at Finite Temperature

Stefan Glocke, Andreas Klümper, and Jesko Sirker 665

25.1 Introduction 665

25.2 Quantum Transfer Matrix Theory 666

25.3 The Method – DMRG Algorithm for the QTM 669

25.4 An Example: The Spin-1/2 Heisenberg Chain with Staggered and Uniform Magnetic Fields 671

25.5 Impurity and Boundary Contributions 672

25.6 Real-Time Dynamics 673

References 676

Part X Concepts of High Performance Computing

26 Architecture and Performance Characteristics of Modern High Performance Computers

Georg Hager and Gerhard Wellein 681

26.1 Microprocessors 682

26.2 Parallel Computing 701

26.3 Conclusion and Outlook 729

References 729

27 Optimization Techniques for Modern High Performance Computers

Georg Hager and Gerhard Wellein 731

27.1 Optimizing Serial Code 732

27.2 Shared-Memory Parallelization 755

27.3 Conclusion and Outlook 766

References 767

Appendix: Abbreviations 769

Index 773

