

# 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**

<i>Wolfhard Janke</i> . . . . .	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**

<i>Detlev Reiter</i> . . . . .	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**

<i>David Tskhakaya</i> . . . . .	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**

<i>Richard D. Sydora</i> . . . . .	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 Xavier 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**  
*Ingo Peschel and Viktor Eisler* . . . . . 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**  
*Eric Jeckelmann* . . . . . 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**  
*Eric Jeckelmann and Holger Benthien* . . . . . 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**  
*Reinhard M. Noack, Salvatore R. Manmana, Stefan Wessel,  
and Alejandro Muramatsu* . . . . . 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**

<i>Ö. Legeza, R.M. Noack, J. Sólyom, and L. Tincani</i> . . . . .	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**

<i>Stefan Glocke, Andreas Klümper, and Jesko Sirker</i> . . . . .	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**

<i>Georg Hager and Gerhard Wellein</i> . . . . .	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**

<i>Georg Hager and Gerhard Wellein</i> . . . . .	731
27.1 Optimizing Serial Code . . . . .	732
27.2 Shared-Memory Parallelization . . . . .	755
27.3 Conclusion and Outlook . . . . .	766
References . . . . .	767

<b>Appendix: Abbreviations</b> . . . . .	769
--	-----

<b>Index</b> . . . . .	773
------------------------	-----





Computational Many-Particle Physics

Fehske, H.; Schneider, R.; Weiße, A. (Eds.)

2008, XV, 780 p., Hardcover

ISBN: 978-3-540-74685-0