

COMPUTATIONAL PHYSICS

Second Edition

JOS THIJS SEN

Kavli Institute of Nanoscience, Delft University of Technology



CAMBRIDGE
UNIVERSITY PRESS

Contents

Preface to the first edition	<i>page xi</i>
Preface to the second edition	<i>xiv</i>
1 Introduction	1
1.1 Physics and computational physics	1
1.2 Classical mechanics and statistical mechanics	1
1.3 Stochastic simulations	4
1.4 Electrodynamics and hydrodynamics	5
1.5 Quantum mechanics	6
1.6 Relations between quantum mechanics and classical statistical physics	7
1.7 Quantum molecular dynamics	8
1.8 Quantum field theory	9
1.9 About this book	9
Exercises	11
References	13
2 Quantum scattering with a spherically symmetric potential	14
2.1 Introduction	14
2.2 A program for calculating cross sections	18
2.3 Calculation of scattering cross sections	25
Exercises	27
References	28
3 The variational method for the Schrödinger equation	29
3.1 Variational calculus	29
3.2 Examples of variational calculations	32
3.3 Solution of the generalised eigenvalue problem	36
3.4 Perturbation theory and variational calculus	37

	Exercises	39
	References	41
4	The Hartree—Fock method	43
4.1	Introduction	43
4.2	The Born—Oppenheimer approximation and the independent-particle method	44
4.3	The helium atom	46
4.4	Many-electron systems and the Slater determinant	52
4.5	Self-consistency and exchange: Hartree—Fock theory	54
4.6	Basis functions	60
4.7	The structure of a Hartree—Fock computer program	69
4.8	Integrals involving Gaussian functions	73
4.9	Applications and results	77
4.10	Improving upon the Hartree—Fock approximation	78
	Exercises	80
	References	87
5	Density functional theory	89
5.1	Introduction	89
5.2	The local density approximation	95
5.3	Exchange and correlation: a closer look	97
5.4	Beyond DFT: one- and two-particle excitations	101
5.5	A density functional program for the helium atom	109
5.6	Applications and results	114
	Exercises	116
	References	119
6	Solving the Schrödinger equation in periodic solids	122
6.1	Introduction: definitions	123
6.2	Band structures and Bloch's theorem	124
6.3	Approximations	126
6.4	Band structure methods and basis functions	133
6.5	Augmented plane wave methods	135
6.6	The linearised APW (LAPW) method	141
6.7	The pseudopotential method	144
6.8	Extracting information from band structures	160
6.9	Some additional remarks	162
6.10	Other band methods	163

Exercises	163
References	167
7 Classical equilibrium statistical mechanics	169
7.1 Basic theory	169
7.2 Examples of statistical models; phase transitions	176
7.3 Phase transitions	184
7.4 Determination of averages in simulations	192
Exercises	194
References	195
8 Molecular dynamics simulations	197
8.1 Introduction	197
8.2 Molecular dynamics at constant energy	200
8.3 A molecular dynamics simulation program for argon	208
8.4 Integration methods: symplectic integrators	211
8.5 Molecular dynamics methods for different ensembles	223
8.6 Molecular systems	232
8.7 Long-range interactions	241
8.8 Langevin dynamics simulation	247
8.9 Dynamical quantities: nonequilibrium molecular dynamics	251
Exercises	253
References	259
9 Quantum molecular dynamics	263
9.1 Introduction	263
9.2 The molecular dynamics method	266
9.3 An example: quantum molecular dynamics for the hydrogen molecule	272
9.4 Orthonormalisation; conjugate gradient and RM-DIIS techniques	278
9.5 Implementation of the Car—Parrinello technique for pseudopotential DFT	289
Exercises	290
References	293
10 The Monte Carlo method	295
10.1 Introduction	295
10.2 Monte Carlo integration	296
10.3 Importance sampling through Markov chains	299

10.4 Other ensembles	310
10.5 Estimation of free energy and chemical potential	316
10.6 Further applications and Monte Carlo methods	319
10.7 The temperature of a finite system	330
Exercises	334
References	335
11 Transfer matrix and diagonalisation of spin chains	338
11.1 Introduction	338
11.2 The one-dimensional Ising model and the transfer matrix	339
11.3 Two-dimensional spin models	343
11.4 More complicated models	347
11.5 Exact diagonalisation of quantum chains	349
11.6 Quantum renormalisation in real space	355
11.7 The density matrix renormalisation group method	358
Exercises	365
References	370
12 Quantum Monte Carlo methods	372
12.1 Introduction	372
12.2 The variational Monte Carlo method	373
12.3 Diffusion Monte Carlo	387
12.4 Path-integral Monte Carlo	398
12.5 Quantum Monte Carlo on a lattice	410
12.6 The Monte Carlo transfer matrix method	414
Exercises	417
References	421
13 The finite element method for partial differential equations	423
13.1 Introduction	423
13.2 The Poisson equation	424
13.3 Linear elasticity	429
13.4 Error estimators	434
13.5 Local refinement	436
13.6 Dynamical finite element method	439
13.7 Concurrent coupling of length scales: FEM and MD	440
Exercises	445
References	446

14 The lattice Boltzmann method for fluid dynamics	448
14.1 Introduction	448
14.2 Derivation of the Navier—Stokes equations	449
14.3 The lattice Boltzmann model	455
14.4 Additional remarks	458
14.5 Derivation of the Navier—Stokes equation from the lattice Boltzmann model	460
Exercises	463
References	464
15 Computational methods for lattice field theories	466
15.1 Introduction	466
15.2 Quantum field theory	467
15.3 Interacting fields and renormalisation	473
15.4 Algorithms for lattice field theories	477
15.5 Reducing critical slowing down	491
15.6 Comparison of algorithms for scalar field theory	509
15.7 Gauge field theories	510
Exercises	532
References	536
16 High performance computing and parallelism	540
16.1 Introduction	540
16.2 Pipelining	541
16.3 Parallelism	545
16.4 Parallel algorithms for molecular dynamics	552
References	556
Appendix A Numerical methods	557
A1 About numerical methods	557
A2 Iterative procedures for special functions	558
A3 Finding the root of a function	559
A4 Finding the optimum of a function	560
A5 Discretisation	565
A6 Numerical quadratures	566
A7 Differential equations	568
A8 Linear algebra problems	590
A9 The fast Fourier transform	598
Exercises	601
References	603

Appendix B Random number generators	605
B1 Random numbers and pseudo-random numbers	605
B2 Random number generators and properties of pseudo-random numbers	606
B3 Nonuniform random number generators	609
Exercises	611
References	612
Index	613