

Graduate Texts in Physics

Philipp O. J. Scherer

# Computational Physics

Simulation of Classical and Quantum  
Systems

*Second Edition*

计算物理学 第2版

Springer

世界图书出版公司  
[www.wpcbj.com.cn](http://www.wpcbj.com.cn)

Philipp O.J. Scherer

# Computational Physics

## Simulation of Classical and Quantum Systems

Second Edition



Springer

## 图书在版编目 ( CIP ) 数据

计算物理学 : 第 2 版 = Computational Physics : Simulation of Classical  
and Quantum Systems Second Edition : 英文 / ( 德 ) P. O. J. 谢勒 ( P. O. J. Scherer )  
著 . —影印本 . —北京 : 世界图书出版公司北京公司 , 2016.10  
ISBN 978-7-5192-1963-5

I . ①计… II . ①P… III . ①计算物理学—英文 IV . ①O411.1

中国版本图书馆 CIP 数据核字 ( 2016 ) 第 255248 号

著 者 : Philipp O. J. Scherer

责任编辑 : 刘 慧 高 蓉

装帧设计 : 任志远

出版发行 : 世界图书出版公司北京公司

地 址 : 北京市东城区朝内大街 137 号

邮 编 : 100010

电 话 : 010-64038355 ( 发行 ) 64015580 ( 客服 ) 64033507 ( 总编室 )

网 址 : <http://www.wpcbj.com.cn>

邮 箱 : [wpcbjst@vip.163.com](mailto:wpcbjst@vip.163.com)

销 售 : 新华书店

印 刷 : 三河市国英印务有限公司

开 本 : 711mm × 1245mm 1/24

印 张 : 20

字 数 : 384 千

版 次 : 2017 年 1 月第 1 版 2017 年 1 月第 1 次印刷

版权登记 : 01-2016-5271

定 价 : 80.00 元

---

版权所有 翻印必究

( 如发现印装质量问题 , 请与所购图书销售部门联系调换 )

# Graduate Texts in Physics

Graduate Texts in Physics publishes new, authoritative, graduate-level textbooks covering the full range of physics, from classical mechanics to quantum field theory. These textbooks are written by leading experts in their fields and are designed to be used by graduate students and researchers alike. The books are written in a clear, concise, and accessible style, making them ideal for use in the classroom or as a reference work. The series includes books on a wide range of topics, including:

- Classical Mechanics
- Quantum Mechanics
- Statistical Mechanics
- Thermodynamics
- Electromagnetism
- Optics
- Acoustics
- Fluid Dynamics
- Plasma Physics
- Particle Physics
- Astrophysics
- Biophysics
- Geophysics
- Environmental Physics
- Medical Physics
- Engineering Physics

**Series Editor:**  
**Professor Richard D. Mattuck**  
 Cavendish Laboratory  
 11 Thompson Avenue  
 Cambridge CB3 0HH, UK  
 mattuck@cam.ac.uk

**Professor William J. Rines**  
 Department of Computer and Electrical Engineering and Technology  
 Imaging Science and Technology Centre  
 Florida Atlantic University  
 777 Glades Road, SE, Room 400  
 Boca Raton, FL 33431, USA  
 wrines@fau.edu

**Professor Susan Scott**  
 Department of Physics  
 Australian National University  
 Science Road  
 Acton 0200, Australia  
 susan.scott@anu.edu.au

**Professor H. Eugene Stanley**  
 Center for Polymer Studies (Department of Physics)  
 Boston University  
 590 Commonwealth Avenue, Boston 02215  
 Boston, MA 02215, USA  
 stanley@bu.edu

**Professor Martin Spatzman**  
 Walter Schottky Institut  
 TU München  
 85748 Garching, Germany  
 spatzman@wsi-munich.de

For further volumes:  
[www.springer.com/series/8431](http://www.springer.com/series/8431)

# Graduate Texts in Physics

Graduate Texts in Physics publishes core learning/teaching material for graduate- and advanced-level undergraduate courses on topics of current and emerging fields within physics, both pure and applied. These textbooks serve students at the MS- or PhD-level and their instructors as comprehensive sources of principles, definitions, derivations, experiments and applications (as relevant) for their mastery and teaching, respectively. International in scope and relevance, the textbooks correspond to course syllabi sufficiently to serve as required reading. Their didactic style, comprehensiveness and coverage of fundamental material also make them suitable as introductions or references for scientists entering, or requiring timely knowledge of, a research field.

## *Series Editors*

### Professor Richard Needs

Cavendish Laboratory  
JJ Thomson Avenue  
Cambridge CB3 0HE, UK  
rn11@cam.ac.uk

### Professor William T. Rhodes

Department of Computer and Electrical Engineering and Computer Science  
Imaging Science and Technology Center  
Florida Atlantic University  
777 Glades Road SE, Room 456  
Boca Raton, FL 33431, USA  
wrhodes@fau.edu

### Professor Susan Scott

Department of Quantum Science  
Australian National University  
Science Road  
Acton 0200, Australia  
susan.scott@anu.edu.au

### Professor H. Eugene Stanley

Center for Polymer Studies Department of Physics  
Boston University  
590 Commonwealth Avenue, Room 204B  
Boston, MA 02215, USA  
hes@bu.edu

### Professor Martin Stutzmann

Walter Schottky Institut  
TU München  
85748 Garching, Germany  
stutz@wsi.tu-muenchen.de

Philipp O.J. Scherer  
Physikdepartment T38  
Technische Universität München  
Garching, Germany

Additional material to this book can be downloaded from <http://extras.springer.com>.

ISSN 1868-4513

ISSN 1868-4521 (electronic)

Graduate Texts in Physics

ISBN 978-3-319-00400-6

ISBN 978-3-319-00401-3 (eBook)

DOI 10.1007/978-3-319-00401-3

Springer Cham Heidelberg New York Dordrecht London

Library of Congress Control Number: 2013944508

© Springer International Publishing Switzerland 2010, 2013

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed. Exempted from this legal reservation are brief excerpts in connection with reviews or scholarly analysis or material supplied specifically for the purpose of being entered and executed on a computer system, for exclusive use by the purchaser of the work. Duplication of this publication or parts thereof is permitted only under the provisions of the Copyright Law of the Publisher's location, in its current version, and permission for use must always be obtained from Springer. Permissions for use may be obtained through RightsLink at the Copyright Clearance Center. Violations are liable to prosecution under the respective Copyright Law.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

While the advice and information in this book are believed to be true and accurate at the date of publication, neither the authors nor the editors nor the publisher can accept any legal responsibility for any errors or omissions that may be made. The publisher makes no warranty, express or implied, with respect to the material contained herein.

Reprint from English language edition:

Computational Physics: Simulation of Classical and Quantum Systems Second Edition

by Philipp O. J. Scherer

Copyright © Springer International Publishing Switzerland 2010, 2013

Springer is a part of Springer Science+Business Media

All Rights Reserved

This reprint has been authorized by Springer Science & Business Media for distribution in China Mainland only and not for export therefrom.

# Preface to the Second Edition

*To Christine*

# Preface to the Second Edition

This textbook introduces the main principles of computational physics, which include numerical methods and their application to the simulation of physical systems. The first edition was based on a one-year course in computational physics where I presented a selection of only the most important methods and applications. Approximately one-third of this edition is new. I tried to give a larger overview of the numerical methods, traditional ones as well as more recent developments. In many cases it is not possible to pin down the “best” algorithm, since this may depend on subtle features of a certain application, the general opinion changes from time to time with new methods appearing and computer architectures evolving, and each author is convinced that his method is the best one. Therefore I concentrated on a discussion of the prevalent methods and a comparison for selected examples. For a comprehensive description I would like to refer the reader to specialized textbooks like “Numerical Recipes” or elementary books in the field of the engineering sciences.

The major changes are as follows.

A new chapter is dedicated to the discretization of differential equations and the general treatment of boundary value problems. While finite differences are a natural way to discretize differential operators, finite volume methods are more flexible if material properties like the dielectric constant are discontinuous. Both can be seen as special cases of the finite element methods which are omnipresent in the engineering sciences. The method of weighted residuals is a very general way to find the “best” approximation to the solution within a limited space of trial functions. It is relevant for finite element and finite volume methods but also for spectral methods which use global trial functions like polynomials or Fourier series.

Traditionally, polynomials and splines are very often used for interpolation. I included a section on rational interpolation which is useful to interpolate functions with poles but can also be an alternative to spline interpolation due to the recent development of barycentric rational interpolants without poles.

The chapter on numerical integration now discusses Clenshaw-Curtis and Gaussian methods in much more detail, which are important for practical applications due to their high accuracy.

Besides the elementary root finding methods like bisection and Newton-Raphson, also the combined methods by Dekker and Brent and a recent extension by Chandrupatla are discussed in detail. These methods are recommended in most text books. Function minimization is now discussed also with derivative free methods, including Brent's golden section search method. Quasi-Newton methods for root finding and function minimizing are thoroughly explained.

Eigenvalue problems are ubiquitous in physics. The QL-method, which is very popular for not too large matrices is included as well as analytic expressions for several differentiation matrices.

The discussion of the singular value decomposition was extended and its application to low rank matrix approximation and linear fitting is discussed.

For the integration of equations of motion (i.e. of initial value problems) many methods are available, often specialized for certain applications. For completeness, I included the predictor-corrector methods by Nordsieck and Gear which have been often used for molecular dynamics and the backward differentiation methods for stiff problems.

A new chapter is devoted to molecular mechanics, since this is a very important branch of current computational physics. Typical force field terms are discussed as well as the calculation of gradients which are necessary for molecular dynamics simulations.

The simulation of waves now includes three additional two-variable methods which are often used in the literature and are based on generally applicable schemes (leapfrog, Lax-Wendroff, Crank-Nicolson).

The chapter on simple quantum systems was rewritten. Wave packet simulation has become very important in theoretical physics and theoretical chemistry. Several methods are compared for spatial discretization and time integration of the one-dimensional Schrödinger equation. The dissipative two-level system is used to discuss elementary operations on a qubit.

The book is accompanied by many computer experiments. For those readers who are unable to try them out, the essential results are shown by numerous figures.

This book is intended to give the reader a good overview over the fundamental numerical methods and their application to a wide range of physical phenomena. Each chapter now starts with a small abstract, sometimes followed by necessary physical background information. Many references, original work as well as specialized text books, are helpful for more deepened studies.

Garching, Germany

February 2013

Philipp O.J. Scherer

# Preface to the First Edition

Computers have become an integral part of modern physics. They help to acquire, store and process enormous amounts of experimental data. Algebra programs have become very powerful and give the physicist the knowledge of many mathematicians at hand. Traditionally physics has been divided into experimental physics which observes phenomena occurring in the real world and theoretical physics which uses mathematical methods and simplified models to explain the experimental findings and to make predictions for future experiments. But there is also a new part of physics which has an ever growing importance. Computational physics combines the methods of the experimentalist and the theoretician. Computer simulation of physical systems helps to develop models and to investigate their properties.

## Computers in Physics

### Experimental Physics

*data collection, storage and processing*

Communication, data transmission  
data storage and data management  
*email, www, ftp*

Numerical maths  
*approximative methods*

Symbolic Computing  
*algebra programs*

Visualisation & presentation  
*Computer graphics, processing of text and images*

Theoretical Physics  
*approximative solutions*

Computational Physics  
*Computer models & experiments*

This book is a compilation of the contents of a two-part course on computational physics which I have given at the TUM (Technische Universität München) for several years on a regular basis. It attempts to give the undergraduate physics students a profound background in numerical methods and in computer simulation methods but is also very welcome by students of mathematics and computational science

who want to learn about applications of numerical methods in physics. This book may also support lecturers of computational physics and bio-computing. It tries to bridge between simple examples which can be solved analytically and more complicated but instructive applications which provide insight into the underlying physics by doing computer experiments.

The first part gives an introduction into the essential methods of numerical mathematics which are needed for applications in physics. Basic algorithms are explained in detail together with limitations due to numerical inaccuracies. Mathematical explanations are supplemented by numerous numerical experiments.

The second part of the book shows the application of computer simulation methods for a variety of physical systems with a certain focus on molecular biophysics. The main object is the time evolution of a physical system. Starting from a simple rigid rotor or a mass point in a central field, important concepts of classical molecular dynamics are discussed. Further chapters deal with partial differential equations, especially the Poisson-Boltzmann equation, the diffusion equation, nonlinear dynamic systems and the simulation of waves on a 1-dimensional string. In the last chapters simple quantum systems are studied to understand e.g. exponential decay processes or electronic transitions during an atomic collision. A two-state quantum system is studied in large detail, including relaxation processes and excitation by an external field. Elementary operations on a quantum bit (qubit) are simulated.

Basic equations are derived in detail and efficient implications are discussed together with numerical accuracy and stability of the algorithms. Analytical results are given for simple test cases which serve as a benchmark for the numerical methods. Many computer experiments are provided realized as Java applets which can be run in the web browser. For a deeper insight the source code can be studied and modified with the free “netbeans”<sup>1</sup> environment.

Garching, Germany  
April 2010

Philipp O.J. Scherer

<sup>1</sup>[www.netbeans.org](http://www.netbeans.org).

# Contents

## Part I Numerical Methods

<b>1</b>	<b>Error Analysis</b>	3
1.1	Machine Numbers and Rounding Errors	3
1.2	Numerical Errors of Elementary Floating Point Operations	6
1.2.1	Numerical Extinction	7
1.2.2	Addition	8
1.2.3	Multiplication	9
1.3	Error Propagation	9
1.4	Stability of Iterative Algorithms	11
1.5	Example: Rotation	12
1.6	Truncation Error	13
1.7	Problems	14
<b>2</b>	<b>Interpolation</b>	15
2.1	Interpolating Functions	15
2.2	Polynomial Interpolation	16
2.2.1	Lagrange Polynomials	17
2.2.2	Barycentric Lagrange Interpolation	17
2.2.3	Newton's Divided Differences	18
2.2.4	Neville Method	20
2.2.5	Error of Polynomial Interpolation	21
2.3	Spline Interpolation	22
2.4	Rational Interpolation	25
2.4.1	Padé Approximant	25
2.4.2	Barycentric Rational Interpolation	27
2.5	Multivariate Interpolation	32
2.6	Problems	33
<b>3</b>	<b>Numerical Differentiation</b>	37
3.1	One-Sided Difference Quotient	37
3.2	Central Difference Quotient	38

3.3	Extrapolation Methods . . . . .	39
3.4	Higher Derivatives . . . . .	41
3.5	Partial Derivatives of Multivariate Functions . . . . .	42
3.6	Problems . . . . .	43
<b>4</b>	<b>Numerical Integration . . . . .</b>	<b>45</b>
4.1	Equidistant Sample Points . . . . .	46
4.1.1	Closed Newton-Cotes Formulae . . . . .	46
4.1.2	Open Newton-Cotes Formulae . . . . .	48
4.1.3	Composite Newton-Cotes Rules . . . . .	48
4.1.4	Extrapolation Method (Romberg Integration) . . . . .	49
4.2	Optimized Sample Points . . . . .	50
4.2.1	Clenshaw-Curtis Expressions . . . . .	50
4.2.2	Gaussian Integration . . . . .	52
4.3	Problems . . . . .	56
<b>5</b>	<b>Systems of Inhomogeneous Linear Equations . . . . .</b>	<b>59</b>
5.1	Gaussian Elimination Method . . . . .	60
5.1.1	Pivoting . . . . .	63
5.1.2	Direct LU Decomposition . . . . .	63
5.2	QR Decomposition . . . . .	64
5.2.1	QR Decomposition by Orthogonalization . . . . .	64
5.2.2	QR Decomposition by Householder Reflections . . . . .	66
5.3	Linear Equations with Tridiagonal Matrix . . . . .	69
5.4	Cyclic Tridiagonal Systems . . . . .	71
5.5	Iterative Solution of Inhomogeneous Linear Equations . . . . .	73
5.5.1	General Relaxation Method . . . . .	73
5.5.2	Jacobi Method . . . . .	73
5.5.3	Gauss-Seidel Method . . . . .	74
5.5.4	Damping and Successive Over-Relaxation . . . . .	75
5.6	Conjugate Gradients . . . . .	76
5.7	Matrix Inversion . . . . .	77
5.8	Problems . . . . .	78
<b>6</b>	<b>Roots and Extremal Points . . . . .</b>	<b>83</b>
6.1	Root Finding . . . . .	83
6.1.1	Bisection . . . . .	84
6.1.2	Regula Falsi (False Position) Method . . . . .	85
6.1.3	Newton-Raphson Method . . . . .	85
6.1.4	Secant Method . . . . .	86
6.1.5	Interpolation . . . . .	87
6.1.6	Inverse Interpolation . . . . .	88
6.1.7	Combined Methods . . . . .	91
6.1.8	Multidimensional Root Finding . . . . .	97
6.1.9	Quasi-Newton Methods . . . . .	98

6.2	Function Minimization . . . . .	99
6.2.1	The Ternary Search Method . . . . .	99
6.2.2	The Golden Section Search Method (Brent's Method) . . . . .	101
6.2.3	Minimization in Multidimensions . . . . .	106
6.2.4	Steepest Descent Method . . . . .	106
6.2.5	Conjugate Gradient Method . . . . .	107
6.2.6	Newton-Raphson Method . . . . .	107
6.2.7	Quasi-Newton Methods . . . . .	108
6.3	Problems . . . . .	110
7	<b>Fourier Transformation . . . . .</b>	113
7.1	Fourier Integral and Fourier Series . . . . .	113
7.2	Discrete Fourier Transformation . . . . .	114
7.2.1	Trigonometric Interpolation . . . . .	116
7.2.2	Real Valued Functions . . . . .	118
7.2.3	Approximate Continuous Fourier Transformation . . . . .	119
7.3	Fourier Transform Algorithms . . . . .	120
7.3.1	Goertzel's Algorithm . . . . .	120
7.3.2	Fast Fourier Transformation . . . . .	121
7.4	Problems . . . . .	125
8	<b>Random Numbers and Monte Carlo Methods . . . . .</b>	127
8.1	Some Basic Statistics . . . . .	127
8.1.1	Probability Density and Cumulative Probability Distribution . . . . .	127
8.1.2	Histogram . . . . .	128
8.1.3	Expectation Values and Moments . . . . .	129
8.1.4	Example: Fair Die . . . . .	130
8.1.5	Normal Distribution . . . . .	131
8.1.6	Multivariate Distributions . . . . .	132
8.1.7	Central Limit Theorem . . . . .	133
8.1.8	Example: Binomial Distribution . . . . .	133
8.1.9	Average of Repeated Measurements . . . . .	134
8.2	Random Numbers . . . . .	135
8.2.1	Linear Congruent Mapping . . . . .	135
8.2.2	Marsaglia-Zamann Method . . . . .	135
8.2.3	Random Numbers with Given Distribution . . . . .	136
8.2.4	Examples . . . . .	136
8.3	Monte Carlo Integration . . . . .	138
8.3.1	Numerical Calculation of $\pi$ . . . . .	138
8.3.2	Calculation of an Integral . . . . .	139
8.3.3	More General Random Numbers . . . . .	140
8.4	Monte Carlo Method for Thermodynamic Averages . . . . .	141
8.4.1	Simple Sampling . . . . .	141
8.4.2	Importance Sampling . . . . .	142
8.4.3	Metropolis Algorithm . . . . .	142
8.5	Problems . . . . .	144

**9 Eigenvalue Problems** . . . . . 147

9.1 Direct Solution . . . . . 148

9.2 Jacobi Method . . . . . 148

9.3 Tridiagonal Matrices . . . . . 150

9.3.1 Characteristic Polynomial of a Tridiagonal Matrix . . . . . 151

9.3.2 Special Tridiagonal Matrices . . . . . 151

9.3.3 The *QL* Algorithm . . . . . 156

9.4 Reduction to a Tridiagonal Matrix . . . . . 157

9.5 Large Matrices . . . . . 159

9.6 Problems . . . . . 160

**10 Data Fitting** . . . . . 161

10.1 Least Square Fit . . . . . 162

10.1.1 Linear Least Square Fit . . . . . 163

10.1.2 Linear Least Square Fit with Orthogonalization . . . . . 165

10.2 Singular Value Decomposition . . . . . 167

10.2.1 Full Singular Value Decomposition . . . . . 168

10.2.2 Reduced Singular Value Decomposition . . . . . 168

10.2.3 Low Rank Matrix Approximation . . . . . 170

10.2.4 Linear Least Square Fit with Singular Value Decomposition . . . . . 172

10.3 Problems . . . . . 175

**11 Discretization of Differential Equations** . . . . . 177

11.1 Classification of Differential Equations . . . . . 178

11.1.1 Linear Second Order PDE . . . . . 178

11.1.2 Conservation Laws . . . . . 179

11.2 Finite Differences . . . . . 180

11.2.1 Finite Differences in Time . . . . . 181

11.2.2 Stability Analysis . . . . . 182

11.2.3 Method of Lines . . . . . 183

11.2.4 Eigenvector Expansion . . . . . 183

11.3 Finite Volumes . . . . . 185

11.3.1 Discretization of fluxes . . . . . 188

11.4 Weighted Residual Based Methods . . . . . 190

11.4.1 Point Collocation Method . . . . . 191

11.4.2 Sub-domain Method . . . . . 191

11.4.3 Least Squares Method . . . . . 192

11.4.4 Galerkin Method . . . . . 192

11.5 Spectral and Pseudo-spectral Methods . . . . . 193

11.5.1 Fourier Pseudo-spectral Methods . . . . . 193

11.5.2 Example: Polynomial Approximation . . . . . 194

11.6 Finite Elements . . . . . 196

11.6.1 One-Dimensional Elements . . . . . 196

11.6.2 Two- and Three-Dimensional Elements . . . . . 197

11.6.3 One-Dimensional Galerkin FEM . . . . . 201

11.7 Boundary Element Method . . . . . 204

<b>12 Equations of Motion</b>	207
12.1 The State Vector	208
12.2 Time Evolution of the State Vector	209
12.3 Explicit Forward Euler Method	210
12.4 Implicit Backward Euler Method	212
12.5 Improved Euler Methods	213
12.6 Taylor Series Methods	215
12.6.1 Nordsieck Predictor-Corrector Method	215
12.6.2 Gear Predictor-Corrector Methods	217
12.7 Runge-Kutta Methods	217
12.7.1 Second Order Runge-Kutta Method	218
12.7.2 Third Order Runge-Kutta Method	218
12.7.3 Fourth Order Runge-Kutta Method	219
12.8 Quality Control and Adaptive Step Size Control	220
12.9 Extrapolation Methods	221
12.10 Linear Multistep Methods	222
12.10.1 Adams-Bashforth Methods	222
12.10.2 Adams-Moulton Methods	223
12.10.3 Backward Differentiation (Gear) Methods	223
12.10.4 Predictor-Corrector Methods	224
12.11 Verlet Methods	225
12.11.1 Liouville Equation	225
12.11.2 Split-Operator Approximation	226
12.11.3 Position Verlet Method	227
12.11.4 Velocity Verlet Method	227
12.11.5 Störmer-Verlet Method	228
12.11.6 Error Accumulation for the Störmer-Verlet Method	229
12.11.7 Beeman's Method	230
12.11.8 The Leapfrog Method	231
12.12 Problems	232

## Part II Simulation of Classical and Quantum Systems

<b>13 Rotational Motion</b>	239
13.1 Transformation to a Body Fixed Coordinate System	239
13.2 Properties of the Rotation Matrix	240
13.3 Properties of $W$ , Connection with the Vector of Angular Velocity	242
13.4 Transformation Properties of the Angular Velocity	244
13.5 Momentum and Angular Momentum	246
13.6 Equations of Motion of a Rigid Body	246
13.7 Moments of Inertia	247
13.8 Equations of Motion for a Rotor	248
13.9 Explicit Methods	248
13.10 Loss of Orthogonality	250
13.11 Implicit Method	251
13.12 Kinetic Energy of a Rotor	255

13.13	Parametrization by Euler Angles . . . . .	255
13.14	Cayley-Klein Parameters, Quaternions, Euler Parameters . . . . .	256
13.15	Solving the Equations of Motion with Quaternions . . . . .	259
13.16	Problems . . . . .	260
<b>14</b>	<b>Molecular Mechanics . . . . .</b>	<b>263</b>
14.1	Atomic Coordinates . . . . .	264
14.2	Force Fields . . . . .	266
14.2.1	Intramolecular Forces . . . . .	267
14.2.2	Intermolecular Interactions . . . . .	269
14.3	Gradients . . . . .	270
14.4	Normal Mode Analysis . . . . .	274
14.4.1	Harmonic Approximation . . . . .	274
14.5	Problems . . . . .	276
<b>15</b>	<b>Thermodynamic Systems . . . . .</b>	<b>279</b>
15.1	Simulation of a Lennard-Jones Fluid . . . . .	279
15.1.1	Integration of the Equations of Motion . . . . .	280
15.1.2	Boundary Conditions and Average Pressure . . . . .	281
15.1.3	Initial Conditions and Average Temperature . . . . .	281
15.1.4	Analysis of the Results . . . . .	282
15.2	Monte Carlo Simulation . . . . .	287
15.2.1	One-Dimensional Ising Model . . . . .	287
15.2.2	Two-Dimensional Ising Model . . . . .	289
15.3	Problems . . . . .	290
<b>16</b>	<b>Random Walk and Brownian Motion . . . . .</b>	<b>293</b>
16.1	Markovian Discrete Time Models . . . . .	293
16.2	Random Walk in One Dimension . . . . .	294
16.2.1	Random Walk with Constant Step Size . . . . .	295
16.3	The Freely Jointed Chain . . . . .	296
16.3.1	Basic Statistic Properties . . . . .	297
16.3.2	Gyration Tensor . . . . .	299
16.3.3	Hookean Spring Model . . . . .	300
16.4	Langevin Dynamics . . . . .	301
16.5	Problems . . . . .	303
<b>17</b>	<b>Electrostatics . . . . .</b>	<b>305</b>
17.1	Poisson Equation . . . . .	305
17.1.1	Homogeneous Dielectric Medium . . . . .	306
17.1.2	Numerical Methods for the Poisson Equation . . . . .	307
17.1.3	Charged Sphere . . . . .	309
17.1.4	Variable $\epsilon$ . . . . .	311
17.1.5	Discontinuous $\epsilon$ . . . . .	313
17.1.6	Solvation Energy of a Charged Sphere . . . . .	314
17.1.7	The Shifted Grid Method . . . . .	314