

<<计算物理学>>

图书基本信息

书名：<<计算物理学>>

13位ISBN编号：9787510032905

10位ISBN编号：7510032903

出版时间：2011-4

出版时间：世界图书出版公司

作者：蒂森

页数：620

版权说明：本站所提供下载的PDF图书仅提供预览和简介，请支持正版图书。

更多资源请访问：<http://www.tushu007.com>

<<计算物理学>>

内容概要

This Second Edition has been fully updated. The wide range of topics covered in the First Edition has been extended with new chapters on finite element methods and lattice Boltzmann simulation. New sections have been added to the chapters on density functional theory, quantum molecular dynamics, Monte Carlo simulation and diagonalisation of one-dimensional quantum systems.

The book covers many different areas of physics research and different computational methodologies, with an emphasis on condensed matter physics and physical chemistry. It includes computational methods such as Monte Carlo and molecular dynamics, various electronic structure methodologies, methods for solving partial differential equations, and lattice gauge theory. Throughout the book, the relations between the methods used in different fields of physics are emphasised. Several new programs are described and these can be downloaded from www.cambridge.org/9780521833462

The book requires a background in elementary programming, numerical analysis and field theory, as well as undergraduate knowledge of condensed matter theory and statistical physics. It will be of interest to graduate students and researchers in theoretical, computational and experimental physics. Jos THIJSEN is a lecturer at the Kavli Institute of Nanoscience at Delft University of Technology.

<<计算物理学>>

作者简介

作者：(荷兰)蒂森 (J.M.Thijssen)

<<计算物理学>>

书籍目录

- preface to the first edition
- preface to the second edition
- 1 introduction
 - 1.1 physics and computational physics
 - 1.2 classical mechanics and statistical mechanics
 - 1.3 stochastic simulations
 - 1.4 electrodynamics and hydrodynamics
 - 1.5 quantum mechanics
 - 1.6 relations between quantum mechanics and classical statistical physics
- 2 quantum scattering with a spherically symmetric potential
 - 2.1 introduction
 - 2.2 a program for calculating cross sections
 - 2.3 calculation of scattering cross sections
 - exercises
 - references
- 3 the variational method for the schr'odinger equation
 - 3.1 variational calculus
 - 3.2 examples of variational calculations
 - 3.3 solution of the generalised eigenvalue problem
 - 3.4 perturbation theory and variational calculus
 - exercises
 - references
- 4 the hartree-fock method
 - 4.1 introduction
 - 4.2 the bom-oppenheimer approximation and the independent-particle method
 - 4.3 the helium atom
 - 4.4 many-electron systems and the slater determinant
 - 4.5 self-consistency and exchange: hartree-fock theory
 - 4.6 basis functions
 - 4.7 the structure of a hartree-fock computer program
 - 4.8 integrals involving gaussian functions
 - 4.9 applications and results
 - 4.10 improving upon the hartree-fock approximation
 - exercises
 - references
- 5 density functional theory
 - 5.1 introduction

<<计算物理学>>

- 5.2 the local density approximation
- 5.3 exchange and correlation: a closer look
- 5.4 beyond dft: one- and two-particle excitations
- 5.5 a density functional program for the helium atom
- 5.6 applications and results
- exercises
- references
- 6 solving the schrodinger equation in periodic solids
 - 6.1 introduction: definitions
 - 6.2 band structures and bloch's theorem
 - 6.3 approximations
 - 6.4 band structure methods and basis functions
 - 6.5 augmented plane wave methods
 - 6.6 the linearised apw (lapw) method
 - 6.7 the pseudopotential method
 - 6.8 extracting information from band structures
 - 6.9 some additional remarks
 - 6.10 other band methods
 - exercises
 - references
- 7 classical equilibrium statistical mechanics
 - 7.1 basic theory
 - 7.2 examples of statistical models; phase transitions
 - 7.3 phase transitions
 - 7.4 determination of averages in simulations
 - exercises
 - references
- 8 Molecular dynamics simulations
 - 8.1 introduction
 - 8.2 molecular dynamics at constant energy
 - 8.3 a molecular dynamics simulation program for argon
 - 8.4 integration methods: symplectic integrators
 - 8.5 molecular dynamics methods for different ensembles
 - 8.6 molecular systems
 - 8.7 long-range interactions
 - 8.8 langevin dynamics simulation
 - 8.9 dynamical quantities: nonequilibrium molecular dynamics
 - exercises
 - references
- 9 quantum molecular dynamics
 - 9.1 introduction
 - 9.2 the molecular dynamics method
 - 9.3 an example: quantum molecular dynamics for the hydrogen molecule
 - 9.4 orthonormalisation; conjugate gradient and rm-diis techniques
 - 9.5 implementation of the car-parrinello technique for

<<计算物理学>>

pseudopotential dft

exercises

references

10 the monte carlo method

10.1 introduction

10.2 monte carlo integration

10.3 importance sampling through markov chains

10.4 other ensembles

10.5 estimation of free energy and chemical potential

10.6 further applications and monte carlo methods

10.7 the temperature of a finite system

exercises

references

11 transfer matrix and diagonalisation of spin chains

11.1 introduction

11.2 the one-dimensional ising model and the transfer matrix

11.3 two-dimensional spin models

11.4 more complicated models

11.5 'exact' diagonalisation of quantum chains

11.6 quantum renormalisation in real space

11.7 the density matrix renormalisation group method

exercises

references

12 quantum monte carlo methods

12.1 introduction

12.2 the variational monte carlo method

12.3 diffusion monte carlo

12.4 path-integral monte carlo

12.5 quantum monte carlo on a lattice

12.6 the monte carlo transfer matrix method

exercises

references

13 the finite element method for partial differential

equations

13.1 introduction

13.2 the poisson equation

13.3 linear elasticity

13.4 error estimators

13.5 local refinement

13.6 dynamical finite element method

13.7 concurrent coupling of length scales: fem and md

exercises

references

14 the lattice boltzmann method for fluid dynamics

14.1 introduction

14.2 derivation of the navier-stokes equations

14.3 the lattice boltzmann model

<<计算物理学>>

- 14.4 additional remarks
- 14.5 derivation of the navier-stokes equation from the lattice boltzmann model
- exercises
- references
- 15 computational methods for lattice field theories
 - 15.1 introduction
 - 15.2 quantum field theory
 - 15.3 interacting fields and renormalisation
 - 15.4 algorithms for lattice field theories
 - 15.5 reducing critical slowing down
 - 15.6 comparison of algorithms for scalar field theory
 - 15.7 gauge field theories
 - exercises
 - references
- 16 high performance computing and parallelism
 - 16.1 introduction
 - 16.2 pipelining
 - 16.3 parallelism
 - 16.4 parallel algorithms for molecular dynamics
 - references
- Appendix a numerical methods
 - A1 about numerical methods
 - A2 iterative procedures for special functions
 - A3 finding the root of a function
 - A4 finding the optimum of a function
 - A5 discretisation
 - A6 numerical quadratures
 - A7 differential equations
 - A8 linear algebra problems
 - A9 the fast fourier transform
 - exercises
 - references
- appendix b random number generators
 - B1 random numbers and pseudo-random numbers
 - B2 random number generators and properties of pseudo-random numbers
 - B3 nonuniform random number generators
 - exercises
 - references
- index

章节摘录

版权页：插图：Now we can define the problems in a more abstract way. It is convenient to consider continuum problems. The candidate solutions (for example the possible conformations) form a phase space, and the merit function has some complicated shape on that space - it contains many valleys and mountains, which can be very steep. The solution we seek corresponds to the lowest valley in the landscape. Note that the landscape is high-dimensional. You may think, naively, that a standard numerical minimum finder can solve this problem for you. However, this is not the case as such an algorithm always needs a starting point, from which it finds the nearest local minimum, which is not necessarily the best you can find in the conformation space. The set of points which would go to one particular local minimum when fed into a steepest descent or other minimum-finder (see Appendix A4) is called the basin of attraction of that minimum. Once we are in the basin of attraction of the global minimum we can easily find this global minimum; the problem is to find its basin of attraction.

<<计算物理学>>

编辑推荐

《计算物理学(英文版)(第2版)》是由世界图书出版公司出版的。

<<计算物理学>>

版权说明

本站所提供下载的PDF图书仅提供预览和简介，请支持正版图书。

更多资源请访问:<http://www.tushu007.com>