

计算物理学



[计算物理学_下载链接1](#)

著者:蒂森

出版者:世界图书出版公司

出版时间:2011-4

装帧:

isbn:9787510032905

《计算物理学(英文版)(第2版)》是一部理论物理研究的计算方法的教程。这是第二版，在第一版的基础上做了大量的更新，内容更加全面。新增加的部分包括，有限元方法，格点boltzmann模拟，密度函数理论，量子分子动力学，monte carlo模拟和一维量子系统的对角化。书中囊括了物理研究的很多不同方面和不同计算方法论。如monte carlo方法和分子模拟动力学以及各种电子结构方法论，偏微分方程解方法，格点规范理论。全书都在强调不同物理场中的方法之间的关系，内容较为简洁明快，具有基本编程，数值分析，场论以及凝聚态理论和统计物理的本科知识背景就可以完全读懂《计算物理学(第2版)》。不管是理论物理，计算物理还是实验物理专业的研究生还是科研人员，《计算物理学(第2版)》都相当有参考价值。目次：导论；具有球对称势的量子散射；schrödinger方程的变分大法；hartree-fock方法；密度函数理论；周期性固态schrödinger方程解法；经典平衡态统计力学；分子动力学模拟；量子分子动力学；monte carlo方法；变换矩阵和自旋链的对角化；量子monte carlo方法，偏微分方程的有限元方法，流体力学的lattice boltzmann方法，格点场论的计算方法；高效能计算和并行法；附：数值法；随机数发生器。

读者对象：物理专业，包括理论物理，计算物理，实验物理的高年级本科生，研究生和

相关的科研人员。

作者介绍:

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 1.7 Quantum molecular dynamics 1.8 Quantum field theory 1.9 About this book Exercises References 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 Schriidinger 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 l-lartree---Fock method 4.1 Introduction 4.2 The Born-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 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 Schriidinger 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 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 References14 The lattice Boltzmann method for fluid dynamics 14.1 Introduction 14.2 Derivation of the Navier-Stokes equations 14.3 The lattice Boltzmann model 14.4 Additional remarks 14.5 Derivation of the Navier-Stokes equation from the lattice Boltzmann model Exercises References15 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 References16 High performance computing and parallelism 16.1 Introduction 16.2 Pipelining 16.3 Parallelism 16.4 Parallel algorithms for molecular dynamics ReferencesAppendix 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 ReferencesAppendix 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 ReferencesIndex

• • • • • (收起)

[计算物理学 下载链接1](#)

标签

计算物理

物理

凝聚态物理

计算力学7

物理-计算物理

评论

公式略多

12年12月28日，开会的时候看陈老师手上拿着一本书，还以为是电子结构。人家刚从伯克利回来，所以俺就凑过去套了下近乎，结果发现不是电子结构~而是这本书。我当时在想这初学者的书还要看吗？陈老师和魏苏怀都发了N篇的PRB了~~~计算物理初级和中级过渡读物。推荐！

[计算物理学 下载链接1](#)

书评

[计算物理学 下载链接1](#)