Computational Methods In Condensed Matter Electronic Structure

LACEY GRIMES

Computer Simulations in Condensed Matter: From Materials to Chemical Biology. Volume 2 Springer Science & Business Media
This volume contains the lectures given at the Third Gordon Godfrey International Workshop on Computational Approaches to Novel Condensed Matter Systems which was held at The University of New South Wales July 12-17, 1993. Lecturers from Asia, Australia, Europe and North America gave a total of twenty-nine lectures which were spread over the five days. Unfortunately we were not able to include in this volume the lectures of S. Das Sarma from the University of Maryland on "Non-Equilibrium Growth as a Self-Organised Phenomenon" due to constraints of time. The workshops have been held annually since 1991 in Sydney, each covering a novel research area in condensed matter physics that is of topical interest. Australia has a strong tradition of research in condensed matter physics. The workshops are jointly organised by the School of Physics at the University of New South Wales (Sydney) and the Department of Theoretical Physics, Research School of Physical Sciences and Engineering at the Australian National University (Canberra). The late Gordon God frey was an Associate Professor of Physics at the University of New South Wales. He bequeathed his estate for the promotion and teaching of theoretical physics within the university. The primary purpose of each workshop is to expose post-graduate students in physics to both informal interaction and formal lectures from recognised international leaders in topical research areas. Past experience has demonstrated again and again that to be informed about a new field there is no substitute for personal contact and interaction.
Computer Simulations Of Molecules And Condensed Matter: From Electronic Structures To Molecular Dynamics Springer Science & Business Media
Computional physics involves the use of computer calculations and simulations to solve physical problems. This book describes computational methods used in theoretical physics with emphasis on condensed matter applications. Coverage begins with an overview of the wide variety of topics and algorithmic approaches studied in this book. The next chapters concentrate on electronic structure calculations, presenting the Hartree-Fock and Density Functional formalisms, and band structure methods. Later chapters discuss molecular dynamics simulations and Monte Carlo methods in classical and quantum physics, with applications to condensed matter and particle field theories. Each chapter details the necessary fundamentals, describes the formation of a sample program, and includes problems that address related analytical and numerical issues. Useful appendices on numerical methods and random number generators are also included. This volume bridges the gap between undergraduate physics and computational research. It is an ideal textbook for graduate students as well as a valuable reference for researchers.
□□□□*{OCLCbr#E5}{OCLCbr#AD}?* World Scientific
The Monte Carlo method is now widely used and commonly accepted as an important and useful tool in solid state physics and related fields. It is broadly recognized that the technique of "computer simulation" is complementary to both analytical theory and experiment, and can significantly

contribute to ad vancing the understanding of various scientific problems. Widespread applications of the Monte Carlo method to various fields of the statistical mechanics of condensed matter physics have already been reviewed in two previously published books, namely Monte Carlo Methods in Statistical Physics (Topics Curro Phys. , Vol. 7, 1st edn. 1979, 2ndedn. 1986) and Applications of the Monte Carlo Method in Statistical Physics (Topics Curro Phys. , Vol. 36, 1st edn. 1984, 2nd edn. 1987). Meanwhile the field has continued its rapid growth and expansion, and applications to new fields have appeared that were not treated at all in the above two books (e. g. studies of irreversible growth phenomena, cellular automata, interfaces, and quantum problems on lattices). Also, new methodic aspects have emerged, such as aspects of efficient use of vector com puters or parallel computers, more efficient analysis of simulated systems con figurations, and methods to reduce critical slowing down at i>hase transitions. Taken together with the extensive activity in certain traditional areas of research (simulation of classical and quantum fluids, of macromolecular materials, of spin glasses and quadrupolar glasses, etc.

Computational Many-Particle Physics Cambridge University Press

This book consists of contributions given at a symposium in honour of Leopold B. Felsen. They represent the state of the art in dealing with electromagnetic fields, their network theory representation, their computation and, finally, with system applications. The network formulation of field problems can improve the problem formulation and also contribute to the solution methodology. Network theory systematic approaches for circuit analysis are based on the separation of the circuit into the connection circuit and the circuit elements. Many applications in science and technology rely on computations of the electromagnetic field in either man-made or natural complex structures. Because different problems have their own combination of geometrical features, materials, scales and frequency ranges, no single method is best suited for handling all possible cases: instead, a combination of methods or hybridization is needed to attain the greatest flexibility and efficiency.

Computational Methods for Solids and Fluids Springer Science & Business Media

Prominent multinational contributors present articles on condensed matter physics, quantum biology and quantum chemistry. Among the topics covered: reactive molecular collisions, density-functional theory, atomic and molecular phenomena in astrophysics, non-Born-Oppenheimer methods, thin films and surfaces.

Experimental and Computational Techniques in Soft Condensed Matter Physics Iop Concise Physics

Over the past several decades, computational approaches to studying strongly-interacting systems have become increasingly varied and sophisticated. This book provides a comprehensive introduction to state-of-the-art quantum Monte Carlo techniques relevant for applications in correlated systems. Providing a clear overview of variational wave functions, and featuring a detailed presentation of stochastic samplings including Markov chains and Langevin dynamics, which are developed into a discussion of Monte Carlo methods. The variational technique is described, from foundations to a detailed description of its algorithms. Further topics discussed include optimisation techniques, real-time dynamics and projection methods, including Green's function, reptation and auxiliary-field Monte Carlo, from basic definitions to advanced algorithms for efficient codes, and the book concludes with recent developments on the continuum space. Quantum Monte Carlo Approaches for Correlated Systems provides an extensive reference for students and researchers working in condensed matter theory or those interested in advanced numerical methods for electronic simulation.

Quantum Monte Carlo Approaches for Correlated Systems Springer Science & Business Media

Looking for the real state of play in computational many-particle physics? Look no further. This book presents an overview of state-of-the-art numerical methods for studying interacting classical and quantum many-particle systems. A broad range of techniques and algorithms are covered, and emphasis is placed on their implementation on modern high-performance computers. This excellent book comes complete with online files and updates allowing readers to stay right up to date.

Computational Approaches in Condensed-Matter Physics Springer

Electronic structure problems are studied in condensed matter physics and theoretical chemistry to provide important insights into the properties of matter. This 2006 graduate textbook describes the main theoretical approaches and computational techniques, from the simplest approximations to the most sophisticated methods. It starts with a detailed description of the various theoretical approaches to calculating the electronic structure of solids and molecules, including density-functional theory and chemical methods based on Hartree-Fock theory. The basic approximations are thoroughly discussed, and an in-depth overview of recent advances and alternative approaches in DFT is given. The second part discusses the different practical methods used to solve the electronic structure problem computationally, for both DFT and Hartree-Fock approaches. Adopting a unique and open approach, this textbook is aimed at graduate students in physics and chemistry, and is intended to improve communication between these communities. It also serves as a reference for researchers entering the field.

Condensed-Matter and Materials Physics Cambridge University Press

Electronic structure problems are studied in condensed matter physics and theoretical chemistry to provide important insights into the properties of matter. This 2006 graduate textbook describes the main theoretical approaches and computational techniques, from the simplest approximations to the most sophisticated methods. It starts with a detailed description of the various theoretical approaches to calculating the electronic structure of solids and molecules, including density-functional theory and chemical methods based on Hartree-Fock theory. The basic approximations are thoroughly discussed, and an in-depth overview of recent advances and alternative approaches in DFT is given. The second part discusses the different practical methods used to solve the electronic structure problem computationally, for both DFT and Hartree-Fock approaches. Adopting a unique and open approach, this textbook is aimed at graduate students in physics and chemistry, and is intended to improve communication between these communities. It also serves as a reference for researchers entering the field.

Computational Many-Particle Physics Springer

This book is the first of several volumes on solids in the Shock Wave Science and Technology Reference Library. This is a unique collection, and the library as a whole sets out to comprehensively and authoritatively cover and review at research level the subject matter with all its ramifications. All the chapters are self-contained and can be read independently of each other, though they are of course thematically interrelated.

Computer Simulation Studies in Condensed Matter Physics III Springer Science & Business Media

This comprehensive collection of lectures by leading experts in the field introduces and reviews all relevant computer simulation methods and their applications in condensed matter systems. Volume 1 is an in-depth introduction to a vast spectrum of computational techniques for statistical mechanical systems of condensed matter. Volume 2 is a collection of state-of-the-art surveys on numerical experiments carried out for a great number of systems.

Electronic Structure Springer

This textbook for graduate students in physics and chemistry describes the theoretical approaches and computational techniques for studying the behavior of electrons. The first part covers the theoretical methods, including both density-functional theory and Hartree-Fock theory and the latter part discusses the different computational methods.

Computational Physics Springer Science & Business Media

Soft condensed matter physics relies on a fundamental understanding at the interface between physics, chemistry, biology, and engineering for a host of materials and circumstances that are related to, but outside, the traditional definition of condensed matter physics. Featuring contributions from leading researchers in the field, this book uniquely discusses both the contemporary experimental and computational manifestations of soft condensed matter systems. From particle tracking and image analysis, novel materials and computational methods, to confocal microscopy and bacterial assays, this book will equip the reader for collaborative and interdisciplinary research efforts relating to a range of modern problems in nonlinear and non-equilibrium systems. It will enable both graduate students and experienced researchers to supplement a more traditional understanding of thermodynamics and statistical systems with knowledge of the techniques used in contemporary investigations. Color versions of a selection of the figures are available at www.cambridge.org/9780521115902.

Electronic Structure Calculations for Solids and Molecules World Scientific

This comprehensive collection of lectures by leading experts in the field introduces and reviews all relevant computer simulation methods and their applications in condensed matter systems. Volume 1 is an in-depth introduction to a vast spectrum of computational techniques for statistical mechanical systems of condensed matter. Volume 2 is a collection of state-of-the-art surveys on numerical experiments carried out for a great number of systems.

Computer Simulation Studies in Condensed-Matter Physics X Springer Nature

Computer Simulation Studies in Condensed-Matter Physics X is devoted to Prof. Masuo Suzuki's ideas, which have made novel, new simulations possible. These proceedings, of the 1997 workshop, comprise three parts that deal with new algorithms, methods of analysis, and conceptual developments. The first part contains invited papers that deal with simulational studies of classical systems. The second of the proceedings is devoted to invited papers on quantum systems, including new results for strongly correlated electron and quantum spin models. The final part contains a large number of contributed presentations.

COMPUTATIONAL APPROACHES IN PH Springer

This book identifies opportunities, priorities, and challenges for the field of condensed-matter and materials physics. It highlights exciting recent scientific and technological developments and their societal impact and identifies outstanding questions for future research. Topics range from the science of modern technology to new materials and structures, novel quantum phenomena, nonequilibrium physics, soft condensed matter, and new experimental and computational tools. The book also addresses structural challenges for the field, including nurturing its intellectual vitality, maintaining a healthy mixture of large and small research facilities, improving the field's integration with other disciplines, and developing new ways for scientists in academia, government laboratories, and industry to work together. It will be of interest to scientists, educators, students, and policymakers.

Nonlinear Systems, Vol. 1 Wiley-Interscience

This volume presents, for the very first time, an exhaustive collection of those modern numerical methods specifically tailored for the analysis of Strongly Correlated Systems. Many novel materials, with functional properties emerging from macroscopic quantum behaviors at the frontier of modern research in physics, chemistry and material science, belong to this class of systems. Any technique is presented in great detail by its own inventor or by one of the world-wide recognized main contributors. The exposition has a clear pedagogical cut and fully reports on the most relevant case study where the specific technique showed to be very successful in describing and enlightening the puzzling physics of a particular strongly correlated system. The book is intended for advanced graduate students and post-docs in the field as textbook and/or main reference, but also for other researchers in the field who appreciate consulting a single, but comprehensive, source or wishes to get acquainted, in a as painless as possible way, with the working details of a specific technique.

Modern Theories of Many-Particle Systems in Condensed Matter Physics National Academies Press

This primer is a comprehensive collection of analytical and numerical techniques that can be used to extract the non-perturbative physics of quantum field theories. The intriguing connection between Euclidean Quantum Field Theories (QFTs) and statistical mechanics can be used to apply Markov Chain Monte Carlo (MCMC) methods to investigate strongly coupled QFTs. The overwhelming amount of reliable results coming from the field of lattice quantum chromodynamics stands out as an excellent example of MCMC methods in QFTs in action. MCMC methods have revealed the non-perturbative phase structures, symmetry breaking, and bound states of particles in QFTs. The applications also resulted in new outcomes due to cross-fertilization with research areas such as AdS/CFT correspondence in string theory and condensed matter physics. The book is aimed at advanced undergraduate students and graduate students in physics and applied mathematics, and researchers in MCMC simulations and QFTs. At the end of this book the reader will be able to apply the techniques learned to produce more independent and novel research in the field.

Strongly Correlated Systems Cambridge University Press

This book provides a relatively complete introduction to the methods used in computational condensed matter. A wide range of electronic structure theories are introduced, including traditional quantum chemistry methods, density functional theory, many-body perturbation theory, and more.

Molecular dynamics simulations are also discussed, with extensions to enhanced sampling and free-energy calculation techniques including umbrella sampling, meta-dynamics, integrated tempering sampling, etc. As a further extension beyond the standard Born-Oppenheimer molecular dynamics, some simulation techniques for the description of quantum nuclear effects are also covered, based on Feynman's path-integral representation of quantum mechanics. The book aims to help beginning graduate students to set up a framework of the concepts they should know before tackling the physical/chemical problems they will face in their research. Contents: Introduction to Computer Simulations of Molecules and Condensed MatterQuantum Chemistry Methods and Density-Functional TheoryPseudopotentials, Full Potential, and Basis SetsMany-Body Green's Function Theory and the GW ApproximationMolecular DynamicsExtension of Molecular Dynamics, Enhanced Sampling and the Free-Energy CalculationsQuantum Nuclear EffectsAppendices: Useful Mathematical RelationsExpansion of a Non-Local FunctionThe Brillouin-Zone IntegrationThe Frequency IntegrationReferencesAcknowledgements Readership: Researchers in computational condensed matter physics. Keywords: Electronic Structures;First-Principle;Molecular Dynamics;Path-IntegralReview: Key Features: Elaboration on a framework of concepts based on the authors' research experiencesIllustrations of methods ranging from electronic structures to molecular dynamicsDetailed explanation of the path-integral method

Computer Simulations in Condensed Matter: From Materials to Chemical Biology. Volume 1 Cambridge University Press

This book is part of a two volume set which presents the analysis of nonlinear phenomena as a long-standing challenge for research in basic and applied science as well as engineering. It discusses nonlinear differential and differential equations, bifurcation theory for periodic orbits and global connections. The integrability and reversibility of planar vector fields and theoretical analysis of classic physical models are sketched. This first volume concentrates on the mathematical theory and computational techniques that are essential for the study of nonlinear science, a second volume deals with real-world nonlinear phenomena in condensed matter, biology and optics.

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