Density Matrix Quantum Monte Carlo Method Spiral Home

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The Monte Carlo Method in Condensed Matter Physics World Scientific
Quantum Monte Carlo has been established as a powerful computational tool to study quantum many-body systems. It has been successfully applied to small atoms and molecules, the electron gas, hydrogen at high pressures, silicon and carbon clusters, solid silicon and jellium surfaces. The importance of quantum Monte Carlo for these systems is the very accurate treatment of electronic correlation and in the case of hydrogen the direct treatment of the zero-point motion of protons. In this thesis we propose a method of generating pseudopotentials from correlated wave functions, based on the properties of the one-body density matrix and its natural orbitals. We used quantum Monte Carlo techniques to investigate the influence of electronic correlation in obtaining the one-body density matrix and natural orbitals of lithium, carbon and neon, and their influence in the generation of pseudopotentials. In the second part of this work we applied quantum Monte Carlo methods for the study of highly inhomogeneous systems, namely metal surfaces. We did a study of jellium surfaces at a range of densities representative of metals in Nature. In this work we were concerned to learn more about the nature of the wave function and correlation effects in such systems. Such understanding is very important in the construction of wave functions for real metals and in the development and improvement of approximations used in density functional theory. We present results for electronic densities, pair correlation functions and surfaces energies. The results obtained in such calculations provide important benchmarks for other methods.
Recent Progress in Many-Body Theories Springer Science & Business Media
The Monte Carlo method is inherently parallel and the extensive and rapid development in parallel computers, computational clusters and grids has resulted in renewed and increasing interest in this method. At the same time there has been an expansion in the application areas and the method is now widely used in many important areas of science including nuclear and semiconductor physics, statistical mechanics and heat and mass transfer.This book attempts to bridge the gap between theory and practice concentrating on modern algorithmic implementation on parallel architecture machines. Although a suitable text for final year postgraduate mathematicians and computational scientists it is principally aimed at the applied scientists: only a small amount of mathematical knowledge is assumed and theorem proving is kept to a minimum, with the main focus being on parallel algorithms development often to applied industrial problems.A selection of algorithms developed both for serial and parallel machines are provided.
An Introduction to Computational Physics Springer Science & Business Media
Monte Carlo methods have been very prominent in computer simulation of various systems in physics, chemistry, biology, and materials science. This book focuses on the discussion and path-integral quantum Monte Carlo methods in many-body physics and provides a concise but complete introduction to the Metropolis algorithm and its applications in these two techniques. To explore the schemes in clarity, several quantum many-body systems are analysed and studied in detail. The book includes exercises to help digest the materials covered. It can be used as a tutorial to learn the discussion and path-integral Monte Carlo or a recipe for developing new research in the reader's own area. Two complete Java programs, one for the discussion Monte Carlo of 4^He clusters on a graphite surface and the other for the path-integral Monte Carlo of cold atoms in a potential trap, are ready for download and adoption.
Quantum Monte Carlo World Scientific
The first textbook to provide a pedagogical examination of the major algorithms used in quantum Monte Carlo simulations.
Quantum Monte Carlo Approaches for Correlated Systems World Scientific
Monte Carlo methods have been a tool of theoretical and computational scientists for many years. In particular, the invention and percolation of the algorithm of Metropolis, Rosenbluth, Rosenbluth, Teller, and Teller sparked a rapid growth of applications to classical statistical mechanics. Although proposals for treatment of quantum systems had been made even earlier, only a few serious calculations had heen carried out. Ruch calculations are generally more consuming of computer resources than for classical systems and no universal algorithm had--or indeed has yet-- emerged. However, with advances in techniques and in sheer computing power, Monte Carlo methods have been used with considerable success in treating quantum fluids and crystals, simple models of nuclear matter, and few-body nuclei. Research at several institutions suggest that they may offer a new approach to quantum chemistry, one that is independent of basis ann yet capable of chemical accuracy. That. Monte Carlo methods can attain the very great precision needed is itself a remarkable achievement. More recently, new interest in such methods has arisen in two new a~as. Particle theorists, in particular K. Wilson, have drawn attention to the rich analogy between quantum field theoty and statistical mechanics and to the merits of Monte Carlo calculations for lattice gauge theories. This has become a rapidly growing sub-field. A related development is associated with lattice problems in quantum physics, particularly with models of solid state systems. The~ is much ferment in the calculation of various one-dimensional problems such as the'Hubbard model.
Quantum Monte Carlo Study of Pseudopotentials and Metal Surfaces Cambridge University Press
This invaluable book consists of 16 chapters written by some of the most notable researchers in the field of quantum Monte Carlo, highlighting the advances made since Lester Jr.'s 1997 monograph with the same title. It may be regarded as the proceedings of the Symposium on Advances in Quantum Monte Carlo Methods held during the Pacifichem meeting in December 2000, but the contributions go beyond what was presented there. Contents:Theory/Algorithm DevelopmentProperties of Ground State Atoms and MoleculesExcited Electronic StatesLarge Systems and ClustersCondensed Matter Readership: Graduate students and researchers in theoretical chemistry, computational physics, theoretical condensed matter physics, applied physics and applied mathematics. Keywords:
Density Matrix Renormalization Group Elsevier
This Springer Handbook of Metrology and Testing presents the principles of Metrology – the science of measurement – and the methods and techniques of Testing – determining the characteristics of a given product – as they apply to chemical and microstructural analysis, and to the measurement and testing of materials properties and performance, including modelling and simulation. The principal motivation for this Handbook stems from the increasing demands of technology for measurement results that can be used globally. Measurements within a local laboratory or manufacturing facility must be able to be reproduced accurately anywhere in the world. The book integrates knowledge from basic sciences and engineering disciplines, compiled by experts from internationally known metrology and testing institutions, and academe, as well as from industry, and conformity-assessment and accreditation bodies. The Commission of the European Union has expressed this as there is no science without measurements, no quality without testing, and no global markets without standards.
Academic Press
Bosons in an Optical Lattice with a Synthetic Magnetic Field (K Kasamatsu); Quantum Simulation Using Exciton-Polaritons and Their Applications Toward Accelerated Optimization Problem Search (T Byrnes, K Yan, K Kusudo, M Fraser and Y Yamamoto); Quantum Simulation Using Ultracold Atoms in Optical Lattices (S Sugawa, S Taie, R Yamazaki, and Y Takahashi); Universality of Integrable Model: Baxter's T-Q Equation, SU(N)/SU(2)N-3 Correspondence and O-Deformed Seiberg-Witten Prepotential (Ta-sheng Tai); Exact Analysis of Correlation Functions of the XXZ Chain (T Deguchi, K Motegi and J Sato); Classical Analogue of Weak Value in Stochastic Process (H Tomita); Scaling of Entanglement Entropy and Hyperbolic Geometry (H Matsueda); From Classical Neural Networks to Quantum Neural

Networks (B Tirozzi); Analysis of Quantum Monte Carlo Dynamics in Infinite-range Ising Spin Systems: Theory and Its Possible Applications (J Inoue); A Method to Control Order of Phase Transition: Invisible States in Discrete Spin Models (R Tamura, S Tanaka and N Kawashima); Quantum Annealing and Quantum Fluctuation Effect in Frustrated Ising Systems (S Tanaka and R Tamura).

Quantum Monte Carlo Methods in Condensed Matter Physics timbyrnes

The technological means now exists for approaching the fundamentallimiting scales of solid state electronics in which a single carrier can, in principle, represent a single bit in an information flow. In this light, the prospect of chemically, or biologically, engineered molccular-scale structures which might support information processing functions has enticed workers for many years. The one common factor in all suggested molecular switches, ranging from the experimentally feasible proton-tunneling structure, to natural systems such as the micro-tubule, is that each proposed structure deals with individual information carrying entities. Whereas this future molecular electronics faces enormous technical challenges, the same limit is already appearing in existing semiconducting quantum wires and small tunneling structures, both superconducting and normal meta! devices, in which the motion of a single eh arge through the tunneling barrier can produce a sufficient voltage change to cut-off further tunneling current. We may compare the above situation with today's Si microelectronics, where each bit is encoded as a very !arge number, not necessarily fixed, of electrons within acharge pulse. The associated reservoirs and sinks of charge carriers may be profitably tapped and manipulated to proviele macro-currents which can be readily amplified or curtailed. On the other band, modern semiconductor ULSI has progressed by adopting a linear scaling principle to the down-sizing of individual semiconductor devices.

Quantum Monte Carlo Methods World Scientific Publishing Company

The use of quantum chemistry for the quantitative prediction of molecular properties has long been frustrated by the technical difficulty of carrying out the needed computations. In the last decade there have been substantial advances in the formalism and computer hardware needed to carry out accurate calculations of molecular properties efficiently. These advances have been sufficient to make quantum chemical calculations a reliable tool for the quantitative interpretation of chemical phenomena and a guide to laboratory experiments. However, the success of these recent developments in computational quantum chemistry is not well known outside the community of practitioners. In order to make the larger community of chemical physicists aware of the current state of the subject, this self-contained volume of Advances in Chemical Physics surveys a number of the recent accomplishments in computational quantum chemistry. This stand-alone work presents the cutting edge of research in computational quantum mechanics. Supplemented with more than 150 illustrations, it provides evaluations of a broad range of methods, including: * Quantum Monte Carlo methods in chemistry * Monte Carlo methods for real-time path integration * The Redfield equation in condensed-phase quantum dynamics * Path-integral centroid methods in quantum statistical mechanics and dynamics * Multiconfigurational perturbation theory-applications in electronic spectroscopy * Electronic structure calculations for molecules containing transition metals * And more Contributors to New Methods in Computational Quantum Mechanics KERSTIN ANDERSSON, Department of Theoretical Chemistry, Chemical Center, Sweden DAVID M. CEPERLEY, National Center for Supercomputing Applications and Department of Physics, University of Illinois at Urbana-Champaign, Illinois MICHAEL A. COLLINS, Research School of Chemistry, Australian National University, Canberra, Australia REINHOLD EGGER, Fakultät für Physik, Universität Freiburg, Freiburg, Germany ANTHONY K. FELTS, Department of Chemistry, Columbia University, New York RICHARD A. FRIESNER, Department of Chemistry, Columbia University, New York MARKUS P. FÜLSCHER, Department of Theoretical Chemistry, Chemical Center, Sweden K. M. HO, Ames Laboratory and Department of Physics, Iowa State University, Ames, Iowa C. H. MAK, Department of Chemistry, University of Southern California, Los Angeles, California PER-ÅKE Malmqvist, Department of Theoretical Chemistry, Chemical Center, Sweden MANUELA MERCHán, Departamento de Química Física, Universitat de Valéncia, Spain LUBOS MITAS, National Center for Supercomputing Applications and Materials Research Laboratory, University of Illinois at Urbana-Champaign, Illinois STEFANO OSS, Dipartimento di Fisica, Università di Trento and Istituto Nazionale di Fisica della Materia, Unità di Trento, Italy KRISTINE PIERLOOT, Department of Chemistry, University of Leuven, Belgium W. THOMAS POLLARD, Department of Chemistry, Columbia University, New York BJÖRN O. ROOS, Department of Theoretical Chemistry, Chemical Center, Sweden LUIS SERRANO-ANDRÉS, Department of Theoretical Chemistry, Chemical Center, Sweden PER E. M. SIEGBAHN, Department of Physics, University of Stockholm, Stockholm, Sweden WALTER THIEL, Institut für Organische Chemie, Universität Zürich, Zürich, Switzerland GREGORY A. VOTH, Department of Chemistry, University of Pennsylvania, Pennsylvania C. Z. Wang, Ames Laboratory and Department of Physi

A Celebration of Physics at the Millennium Arcler Press

On August 20, 2015, a symposium at Lawrence Livermore National Laboratory was held in honor of Berni J. Alder's 90th birthday. Many of Berni's scientific colleagues and collaborators, former students, and post-doctoral fellows came to celebrate and honor Berni and the ground-breaking scientific impact of his many discoveries. This proceedings volume includes contributions from Berni's collaborators and covers a range of topics, including the melting transition in the 2D hard disk system, non-equilibrium fluid relaxation, the role of fluctuations in hydrodynamics, glass transitions, molecular dynamics of dense fluids, shock-wave and finite-strain equation of state relationships, and applications of quantum mechanics in pattern recognition.

Quantum Optics VI Cambridge University Press

The quantum world obeys logic at odds with our common sense intuition. This weirdness is directly displayed in recent experiments juggling with isolated atoms and photons. They are reviewed in this book, combining theoretical insight and experimental description, and providing useful illustrations for learning and teaching of quantum mechanics.

Progress in Computational Physics of Matter World Scientific

The aim of the book is to describe some of the recent advances, through computer simulation in a broad sense, in the understanding of the complex processes occurring in solids and liquids. The rapid growth of computer power, including the new parallel processors, has stimulated a ferment of new theoretical and computational ideas, which have been developed in particular by the authors in a pluriennal research project supported by Consiglio Nazionale delle Ricerche (CNR) for the development of novel software for large scale computations. The book will cover advances in ab initio (Car-Parrinello) molecular dynamics, quantum monte carlo simulations, self-consistent density functional computation of electronic states, classical molecular dynamics simulation of thermodynamic processes, chemical reactions and transport properties. Besides the description of the results of these techniques in leading edge applications, the book will address specific aspects of the algorithms and software which have been developed by the authors in order to implement in an efficient way the new theoretical advances in these computationally intensive problems. These aspects which are generally not discussed in any detail in the literature, can be of great help for newcomers in the field. Contents:Ab-Initio Molecular Dynamics Simulation of Structural Phase Transitions (P Focher & G Chiarotti)Boson Many-Body Problem: Progress in Variational Monte Carlo Computations (L Reatto)Monte Carlo Variational Theory for Fermions (M H Kalos & L Reatto)Recent Developments of Device Simulation Tools for Parallel Processing (M Saraniti & P Lugli)Simulation of Classical and Quantum Activated Processes in the Condensed Phase (G Ciccotti et al.)‘Ab- Initio” Calculations of Electronic Properties of Metallic Solid Solutions (E Bruno et al.)Ab-Initio Calculation of the Electronic (Valence and Core) and Optical Properties of Interfaces (S Ossicini & O Bisi) Readership: Condensed matter physicists, materials science researchers and chemical physicists. keywords: “This is a very good book containing some important approaches to Computational Physics in Condensed Matter. It offers readers pointed explanations on Computational Methods and its application, at the most appropriate stages.” Bulletin of Japan Physical Society

Semiconductor Quantum Dots World Scientific

It is an indisputable fact that computational physics form part of the essential landscape of physical science and physical education. When writing such a book, one is faced with numerous decisions, e. g. : Which topics should be included? What should be assumed about the readers’ prior knowledge? How should balance be achieved between numerical theory and physical application? This book is not elementary. The reader should have a background in qu- tum physics and computing. On the other way the topics discussed are not addressed to the specialist. This work bridges hopefully the gap between - vanced students, graduates and researchers looking for computational ideas beyond their fence and the specialist working on a special topic. Many imp- tant topics and applications are not considered in this book. The selection is of course a personal one and by no way exhaustive and the material presented obviously reflects my own interest. What is Computational Physics? During the past two decades computational physics became the third fun- mental physical discipline. Like the ‘traditional partners’ experimental physics and theoretical physics, computational physics is not restricted to a special area, e. g. , atomic physics or solid state physics. Computational physics is a meth- ical ansatz useful in all subareas and not necessarily restricted to physics. Of course this methods are related to computational aspects, which means nume- cal and algebraic methods, but also the interpretation and visualization of huge amounts of data.

Electron Correlations and Materials Properties 2 Cambridge University Press

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.

Statistical Mechanics: Algorithms and Computations Springer Science & Business Media

This advanced textbook provides an introduction to the basic methods of computational physics.

Methods, Software and Applications OUP USA

Monte Carlo methods are a class of computational algorithms for simulating the behavior of a wide range of various physical and mathematical systems (with many variables). Their utility has increased with general availability of fast computers, and new applications are continually forthcoming. The basic concepts of Monte Carlo are both simple and straightforward and rooted in statistics and probability theory, their defining characteristic being that the methodology relies on random or pseudo-random sequences of numbers. It is a technique of numerical analysis based on the approximate solution of a problem using repeated sampling experiments and observing the proportion of times a given property is satisfied. The term Monte Carlo was first used to describe calculational methods based on chance in the 1940s, but the methods themselves preceded the term by as much as a century. Quantum Monte Carlo (QMC) first appeared in 1982 and similarly was preceded by development of the related calculational methodology. The success of QMC methods over the past few decades has been remarkable, and this book will clearly demonstrate that success in its discussion of applications. For isolated molecules, the basic material of chemistry, QMC methods have produced exact solutions of the Schroedinger equation for very small systems and the most accurate solutions available for very large systems. The range of applications is impressive: folding of protein molecules, interactions in liquids, structure modeling in crystals and enzymes, quantum dots, designing heat shields and aerodynamic forms, architecture, design, business and economics, and even cinema and video games (3D modeling). This book takes a similar approach to Henry Schaefers classic book Quantum Chemistry (OUP, 1984 now a Dover edition), collecting summaries of some of the most important papers in the quantum Monte Carlo literature, tying everything together with analysis and discussion of applications. Quantum Monte Carlo is a reference book for quantum Monte Carlo applications, belonging near the desk of every quantum chemist, physicist, and a wide range of scientists and engineers across many disciplines, destined to become a classic.

Geometrically Constructed Markov Chain Monte Carlo Study of Quantum Spin-phonon Complex Systems Springer Science & Business Media

This book reviews recent developments in the field of polarons, starting with the basics and covering a number of active directions of research. It integrates theory and experimental results.

Advances In The Computational Sciences - Proceedings Of The Symposium In Honor Of Dr Berni Alder's 90th Birthday World Scientific

This edition has been fully updated with several new sections and chapters. It covers many different areas of physics research and different computational methodologies. Throughout the book the relations between the methods used in different fields of physics are emphasised.

Quantum Monte Carlo Simulations of Ultracold Bosons in a Double Well 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.

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