Density Matrix Quantum Monte Carlo Method Spiral Home

This book had its origins in lectures presented at EPFL, Lausanne, during two separate visits (the most recent being to IRRMA). The author is most grateful to Professors A. Baldereschi, R. Car, and A. Quattropani for making these visits possible, and for the splendidly stimulating environment provided. Professors S. Baroni and R. Resta also influenced considerably the presentation of material by constructive help and comments. Most importantly, Chapters 4 and 5 were originally prepared for a review article by Professor G. Senatore, then at Pavia and now in Trieste, and myself for Reviews of Modem Physics (1994). In the 'course of this collaboration, he has taught me a great deal, especially about quantum Monte Carlo procedures, and Chapter 5 is based directly on this review article. Also in Chapter 4, my original draft on Gutzwiller's method has been transformed by his deeper understanding; again this is reflected directly in Chapter 4; especially in the earlier sections. In addition to the above background, it is relevant here to point out that, as a backcloth for the present, largely "state of the art," account, there are two highly relevant earlier books: The Many-body Problem in Quantum Mechanics with W.

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.

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
This is the second in a series of "International Workshops on Electron Correlations and Materials Properties. " The aim of this series of workshops is to provide a periodic (triennial) and in-depth assessment of advances in the study and understanding of the effects that electron-electron interactions in solids have on the determination of measurable properties of materials. The workshop is structured to include exposure to experimental work, to phenomenology, and to ab initio theory. Since correlation effects are pervasive the workshop aims to concentrate on the identification of promising developing methodology, experimental and theoretical, addressing the most critical frontier issues of electron correlations on the properties of materials. This series of workshops is distinguished from other topical meetings and conferences in that it strongly promotes an interdisciplinary approach to the study of correlations, involving the fields of quantum chemistry, physics, and materials science. The First Workshop was held June 28-July 3, 1998, and a proceedings of the workshop was published by KluwerlPlenum. The Second Workshop was held June 24- 29,2001, and this volume contains the proceedings of that scientific meeting. Through the publications of proceedings, the workshop attempts to disseminate the information gathered during the discussions held at the Workshop to the wider scientific community, and to establish a record of advances in the field.

The first textbook to provide a pedagogical examination of the major algorithms used in quantum Monte Carlo simulations.
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.
Strongly correlated nanostructures and lattices ofelectrons are studied when these systems reside in a steady-state nonequilibrium. Much of the work done to date has made use of the nonequilibrium real-time Keldysh Green function technique. These methods include: the Keldysh Green function perturbation theory, time-dependent numerical renormalization group, density matrix renormalization group, and diagrammatic quantum Monte Carlo. In the special case of steady-state nonequilibrium we construct an imaginary-time theory. The motivation to do this is simple: there exist an abundant number of well-established strongly correlated computational solvers for imaginary-time theory and perturbation theory on the imaginary-time contour is much more straightforward than that of the real-time contour. The first model system we focus on is a strongly interacting quantum dot situated between source and drainelectron reservoirs.^The steady-state nonequilibrium boundary condition is established by applying a voltage bias Φ across the reservoirs, in turn modifying the chemical potentials of the leads. For a symmetric voltage drop we have$\mu_{source}=\Phi/2$ and $\mu_{drain}=-\Phi/2$. The dynamics of the electrons are governed by the Hamiltonian $\hat{\mathcal{H}}$ which is inherently independent of the imbalance in the source and drain chemical potentials. The statistics though are determined by the operator $\hat{\mathcal{H}}-\hat{\mathcal{Y}}$, where $\hat{\mathcal{Y}}$ imposes the nonequilibrium boundary condition. We show that it is possible to construct a single effective Hamiltonian $\hat{\mathcal{K}}$ able to describe both the dynamics and statistics of the system. Upon formulating the theory we explicitly show that it is consistent with the real-time Keldysh theory both formally and through an example using perturbation theory.^In these systems there exists a strong interplay between the interactions and nonequilibrium leading to novel nonperturbative phenomena. Therefore, we combine our theory with the Hirsch-Fye quantum Monte Carlo algorithm to study these effects. We then propose a nonequilibrium Hubbard model in the special limit of infinite dimensions (dynamical mean-field theory) where the problem is reduced to solving a self consistent nonequilibrium impurity model. The final chapter concentrates on electron spin and charge filtering through a quantum dot embedded Aharonov-Bohm interferometer.
In this thesis, novel Monte Carlo methods for precisely calculating the critical phenomena of the effectively frustrated quantum spin system are developed and applied to the critical phenomena of the spin-Peierls systems. Three significant methods are introduced for the first time: a new optimization algorithm of the Markov chain transition kernel based on the geometric weight-allocation approach, the extension of the worm (directed-loop) algorithm to nonconserved particles, and the combination with the level spectroscopy. Utilizing these methods, the phase diagram of the one-dimensional XXZ spin-Peierls system is elucidated. Furthermore, the multi-chain and two-dimensional spin-Peierls systems with interchain lattice interaction are investigated. The unbiased simulation shows that the interesting quantum phase transition between the 1D-like liquid phase and the macroscopically-

degenerated dimer phase occurs on the fully-frustrated parameter line that separates the doubly-degenerated dimer phases in the two-dimensional phase diagram. The spin-phonon interaction in the spin-Peierls system introduces the spin frustration, which usually hinders the quantum Monte Carlo analysis, owing to the notorious negative sign problem. In this thesis, the author has succeeded in precisely calculating the critical phenomena of the effectively frustrated quantum spin system by means of the quantum Monte Carlo method without the negative sign.

Focusing on the purely theoretical aspects of strongly correlated electrons, this volume brings together a variety of approaches to models of the Hubbard type - i.e., problems where both localized and delocalized elements are present in low dimensions. The chapters are arranged in three parts. The first part deals with two of the most widely used numerical methods in strongly correlated electrons, the density matrix renormalization group and the quantum Monte Carlo method. The second part covers Lagrangian, Functional Integral, Renormalization Group, Conformal, and Bosonization methods that can be applied to one-dimensional or weakly coupled chains. The third part considers functional derivatives, mean-field, self-consistent methods, slave-bosons, and extensions.

Warm Dense Matter (WDM) occupies a loosely defined region of phase space intermediate between solid, liquid, gas, and plasma, and typically shares characteristics of two or more of these phases. WDM is generally associated with the combination of strongly coupled ions and moderately degenerate electrons, and careful attention to quantum physics and electronic structure is essential. The lack of a small perturbation parameter greatly limits approximate attempts at its accurate description. Since WDM resides at the intersection of solid state and high energy density physics, many high energy density physics (HEDP) experiments pass through this difficult region of phase space. Thus, understanding and modeling WDM is key to the success of experiments on diverse facilities. These include the National Ignition Campaign centered on the National Ignition Facility (NIF), pulsed-power driven experiments on the Z machine, ion-beam-driven WDM experiments on the NDCX-II, and fundamental WDM research at the Linear Coherent Light Source (LCLS). Warm Dense Matter is also ubiquitous in planetary science and astrophysics, particularly with respect to unresolved questions concerning the structure and age of the gas giants, the nature of exosolar planets, and the cosmochronology of white dwarf stars. In this book we explore established and promising approaches to the modeling of WDM, foundational issues concerning the correct theoretical description of WDM, and the challenging practical issues of numerically modeling strongly coupled systems with many degrees of freedom.

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 Iimit 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.

An up-to-date account of this cutting-edge research in a consistent and understandable framework, of special interest to experts in other areas of electronic structure and/or quantum many-body theory. It will serve equally well as a self-contained guide to learning about reduced density matrices either through self-study or in a classroom as well as an invaluable resource for understanding the critical advancements in the field.

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 Optics VI documents the most recent theoretical and experimental developments in this field, with particular emphasis on atomic optics and interferometry, which is a new and rapidly developing area of research. New methods for quantum-noise reduction are also covered.

The present volume contains the text of the invited talks delivered at the Eighth International Conference on Recent Progress in Many-Body Theories held at SchloB Seggau, Province of Styria, Austria, during the period August 22-26, 1994. The pro ceedings of the Fifth Conference (Oulu, Finland 1987), the Sixth Conference (Arad, Israel 1989) and the Seventh Conference (Minneapolis, USA 1991) have been published. by Plenum as the first three volumes of this series.

Papers from the First Conference (Trieste, Italy 1978) comprise Nuclear Physics volume A328, Nos. 1 and 2, the Second Conference (Oaxtepec, Mexico 1979) was published by Springer-Verlag as volume 142 of "Lecture Notes in Physics," entitled "Recent Progress in Many Body Theories." Vol ume 198 of the same series contains the papers from the Third Conference (Altenberg, 1983). These volumes intend to cover a broad spectrum of current research topics in physics that benefit from the application of many-body theories for their elucidation. At the same time there is a focus on the development and refinement of many-body methods. One of the major aims of the conference series has been to foster the exchange of ideas among physicists working in such diverse areas as nuclear physics, quantum chemistry, complex systems, lattice Hamiltonians, quantum fluids and condensed matter physics. The present volume contains contributions from all these areas. th The conference was dedicated on the occasion of Ludwig Boltzmann's 150 birthday.

This book reviews recent developments of quantum Monte Carlo methods and some remarkable applications to interacting quantum spin systems and strongly correlated electron systems. It contains twenty-two papers by thirty authors. Some of the features are as follows. The first paper gives the foundations of the standard quantum Monte Carlo method, including some recent results on higher-order decompositions of exponential operators and ordered exponentials. The second paper presents a general review of quantum Monte Carlo methods used in the present book. One of the most challenging problems in the field of quantum Monte Carlo techniques, the negative-sign problem, is also discussed and new methods proposed to partially overcome it. In addition, low-dimensional quantum spin systems are studied. Some interesting applications of quantum Monte Carlo methods to fermion systems are also presented to investigate the role of strong correlations and fluctuations of electrons and to clarify the mechanism of high-c superconductivity. Not only thermal properties but also quantum-mechanical ground-state properties have been studied by the projection technique using auxiliary fields. Further, the Haldane gap is confirmed by numerical calculations. Active researchers in the forefront of condensed matter physics as well as young graduate students who want to start learning the quantum Monte Carlo methods will find this book useful.

Quantum Monte-Carlo methods represent a systematic alternative to the diagonalization of the Hamiltonian. They are generalizations of the classical Monte Carlo methods to quantum statistical physics and are based on path integral formulation of quantum mechanics. In such way, the many-body problem is reduced to a set of many one-body problems describing independent particles that casually walk in fluctuating external fields. In this way, exact wave functions are restored by statistically averaging independent-particle states.The book begins with the Section 1 providing a brief introduction to the Monte Carlo method and its historical origin, the basilar statistical concepts. Moreover, some of the future impacts of Quantum Monte Carlo techniques in the field of ab initio methods is explored. Section 2 discusses a

new application of variational Monte Carlo method that can describe the compression effect for the helium atom, a new variational Monte Carlo approach based on the Krylov subspace for large-scale shell-model calculations, and a comparison between the variational Monte Carlo and the diffusion Monte Carlo in a study of the Lanthanum atom. Section 3 present recent works about the auxiliary-field quantum Monte Carlo method, also known in nuclear physics as the shell model Monte Carlo method. In particular, applications of the method in heavy nuclei and honeycomb lattice are discussed. Finally, the last Section 4 focuses on path integral representation of Wigner functions, on constrained path quantum Monte Carlo methods and on a new quantum Monte Carlo scheme able to directly sample the full density matrix of a many-body system.

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.

We present path integral ground state (PIGS) quantum Monte Carlo calculations for the ground state (T = 0) properties of repulsively interacting bosons in a three-dimensional external double well potential over a range of interaction strengths and potential parameters. We focus our calculations on ground state number statistics and the one-body density matrix in order to understand the level of squeezing and fragmentation that the system exhibits as a function of interaction strength, and we compare our PIGS results to both a standard and an improved two-mode model and a recently-proposed eight-mode model. In general, the various models agree with the PIGS simulations for weak interactions, but the full quantum Monte Carlo treatment is required to correctly predict the amount of squeezing and fragmentation

exhibited for strong interactions. One novel and somewhat surprising result from our simulations involves the relationship between squeezing and interaction strength: rather than a monotonic relationship between these quantities, we find that for certain double well barrier heights the squeezing increases as a function of interaction strength until it reaches a maximum, after which it decreases again. We also see a similar relationship between fragmentation and interaction strength. We propose novel physical mechanisms to account for this behavior.

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.

Semiconductor Quantum Dots presents an overview of the background and recent developments in the rapidly growing field of ultrasmall semiconductor microcrystallites, in which the carrier confinement is sufficiently strong to allow only quantized states of the electrons and holes. The main emphasis of this book is the theoretical analysis of the confinement induced modifications of the optical and electronic properties of quantum dots in comparison with extended materials. The book develops the theoretical background material for the analysis of carrier quantum-confinement effects, introduces the different confinement regimes for relative or center-of-mass motion quantization of the electron-hole-pairs, and gives an overview of the best approximation schemes for each regime. A detailed discussion of the carrier states in quantum dots is presented and surface polarization instabilities are analyzed, leading to the self-trapping of carriers near the surface of the dots. The influence of spin-orbit coupling on the quantum-confined carrier states is discussed. The linear and nonlinear optical properties of small and large quantum dots are studied in detail and the influence of the quantum-dot size distribution in many realistic samples is outlined. Phonons in quantum dots as well as the influence of external electric or magnetic fields are also discussed. Last but not least the recent developments dealing with regular systems of quantum dots are also reviewed. All things included, this is an important piece of work on semiconductor quantum dots not to be dismissed by serious researchers and physicists.

Here, we study the phase diagram of the one-dimensional bosonic Hubbard model with contact (U) and near neighbor (V) interactions focusing on the gapped Haldane insulating (HI) phase which is characterized by an exotic nonlocal order parameter. The parameter regime (U, V and [mu]) where this phase exists and how it competes with other phases such as the supersolid (SS) phase, is incompletely understood. We use the Stochastic Green Function quantum Monte Carlo algorithm as well as the density matrix renormalization group to map out the phase diagram. The HI exists only at = 1, the SS phase exists for a very wide range of parameters (including commensurate fillings) and displays power law decay in the one body Green function were our main conclusions. Additionally, we show that at fixed integer density, the system exhibits phase separation in the (U, V) plane.

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.

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:

Nonequilibrium hot charge carriers play a crucial role in the physics and technology of semiconductor nanostructure devices. This book, one of the first on the topic, discusses fundamental aspects of hot carriers in quasi-two-dimensional systems and the impact of these carriers on semiconductor devices. The work will provide scientists and device engineers with an authoritative review of the most exciting recent developments in this rapidly moving field. It should be read by all those who wish to learn the fundamentals of contemporary ultra-small, ultra-fast semiconductor devices. Topics covered include Reduced dimensionality and quantum wells Carrier-phonon interactions and hot phonons Femtosecond optical studies of hot carrier Ballistic transport Submicron and resonant tunneling devices

This book presents tutorial overviews for many applications of variational methods to molecular modeling. Topics discussed include the Gibbs-Bogoliubov-Feynman variational principle, square-gradient models, classical density functional theories, self-consistent-field theories, phase-field methods, Ginzburg-Landau and Helfrich-type phenomenological models, dynamical density functional theory, and variational Monte Carlo methods. Illustrative examples are given to facilitate understanding of the basic concepts and quantitative prediction of the properties and rich behavior of diverse many-body systems ranging from inhomogeneous fluids, electrolytes and ionic liquids in micropores, colloidal dispersions, liquid crystals, polymer blends, lipid membranes, microemulsions, magnetic materials and high-temperature superconductors. All chapters are written by leading experts in the field and illustrated with tutorial examples for their practical applications to specific subjects. With emphasis placed on physical understanding rather than on rigorous mathematical derivations, the content is accessible to graduate students and researchers in the broad areas of materials science and engineering, chemistry, chemical and biomolecular engineering, applied mathematics, condensed-matter physics, without specific training in theoretical physics or calculus of variations.

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.

Quantum Monte Carlo Study of Pseudopotentials and Metal Surfaces

This book discusses the computational approach in modern statistical physics, adopting simple language and an attractive format of many illustrations, tables and printed algorithms. The discussion of key subjects in classical and quantum statistical physics will appeal to students, teachers and researchers in physics and related sciences. The focus is on orientation with implementation details kept to a minimum. - ;This book discusses the computational approach in modern statistical physics in a clear and accessible way and demonstrates its close relation to other approaches in theoretical physics. Individual chapters focus on subjects as diverse as the hard sphere liquid, classical spin models, single quantum particles and Bose-Einstein condensation. Contained within the chapters are in-depth discussions of algorithms, ranging from basic enumeration methods to modern Monte Carlo techniques. The emphasis is on orientation, with discussion of implementation details kept to a minimum. Illustrations, tables and concise printed algorithms convey key information, making the material very accessible. The book is completely self-contained and graphs and tables can readily be reproduced, requiring minimal computer code. Most sections begin at an elementary level and lead on to the rich and difficult problems of contemporary computational and statistical physics. The book will be of interest to a wide range of students, teachers and researchers in physics and the neighbouring sciences. An accompanying CD allows incorporation of the book's content (illustrations, tables, schematic programs) into the reader's own presentations. - ;'This book is the best one I have reviewed all year.' Alan Hinchliffe, Physical Sciences Educational Reviews -

In recent years there has been a considerable growth in interest in Monte Carlo methods, and quantum Monte Carlo methods in particlular. Clearly, the ever-increasing computational power available to researchers, has stimulated the development of improved algorithms, and almost all fields in computational physics and chemistry are affected by their

applications. Here we just mention some fields that are covered in the lecture notes contained in this volume, viz. electronic structure studies of atoms, molecules and solids, nuclear structure, and low- or zero-temperature studies of strongly-correlated quantum systems, both of the continuum and lattice variety, and cooperative phenomena in classical systems. Although each area of application may have its own peculiarities, requiring specialized solutions, all share the same basic methodology. It was with the intention of bringing together researchers and students from these various areas that the NATO Advanced Study Institute on Quantum Monte Carlo Methods in Physics and Chemistry was held at Cornell University from 12 to 24 July, 1998. This book contains material presented at the Institute in a series of mini courses in quantum Monte Carlo methods. The program consisted of lectures predominantly of a pedagogical nature, and of more specialized seminars. The levels varied from introductory to advanced, and from basic methods to applications; the program was intended for an audience working towards the Ph.D. level and above. Despite the essentially pedagogic nature of the Institute, several of the lectures and seminars contained in this volume present recent developments not previously published.

The 20th century has been the century of unparalleled scientific advances fuelled primarily by discoveries made by physicists. The century also represents the life span of the American Physical Society, not coincidentally, and to celebrate both its own centennial and this remarkable century, the APS has prepared this book highlighting the seminal discoveries of the 20th century, with invited articles by the world's most eminent living physicists, including 12 physics Nobel Prize winners. Some 40 chapters cover a broad range of topics in physics written in an engaging and personal style. While the technical level is high, these are not review articles, but rather perspectives on discoveries written by those scientists most closely associated with the original work, as well as future directions of research.

These proceedings cover the most recent developments in the fields of high temperature superconductivity, magnetic materials and cold atoms in traps. Special emphasis is given to recently developed numerical and analytical methods, such as effective model Hamiltonians, density matrix renormalization group as well as quantum Monte Carlo simulations. Several of the contributions are written by the pioneers of these methods.

Numerical results for ground-state and excited-state properties (energies, double occupancies, and Matsubara-axis self-energies) of the single-orbital Hubbard model on a two-dimensional square lattice are presented, in order to provide an assessment of our ability to compute accurate results in the thermodynamic limit. Many methods are employed, including auxiliary-field quantum Monte Carlo, bare and bold-line diagrammatic Monte Carlo, method of dual fermions, density matrix embedding theory, density matrix renormalization group, dynamical cluster approximation, diffusion Monte Carlo within a fixed-node approximation, unrestricted coupled cluster theory, and multireference projected Hartree-Fock

methods. Comparison of results obtained by different methods allows for the identification of uncertainties and systematic errors. The importance of extrapolation to converged thermodynamic-limit values is emphasized. Furthermore, cases where agreement between different methods is obtained establish benchmark results that may be useful in the validation of new approaches and the improvement of existing methods.

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.

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).

Advances in Quantum Chemistry presents surveys of current topics in this rapidly developing field one that has emerged at the cross section of the historically established areas of mathematics, physics, chemistry, and biology. It features detailed reviews written by leading international researchers. In this volume the readers are presented with an exciting combination of themes. Presents surveys of current topics in this rapidly-developing field that has emerged at the cross section of the historically established areas of mathematics, physics, chemistry and biology Features detailed reviews written by leading international researchers

This invaluable book deals with the many-electron theory of the solid state. Mastery of the material in it will equip the reader for research in areas such as high-temperature superconductors and the fractional quantum Hall effect. The whole book has been designed to provide the diligent reader with a wide variety of approaches to many-electron theory.The level of the book is suitable for research workers and higher-degree students in a number of disciplines, embracing theoretical physics, materials science and solid-state chemistry. It should be useful not only to theorists in these areas but also to experimental scientists who desire to orient their programmes to address outstanding questions raised by many-body theory.

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.

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