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*Progress in Computational Physics of Matter* World Scientific

In recent years there has been a considerable growth in interest in Monte Carlo methods, and quantum Monte Carlo methods in particular. 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.

*Quantum Monte Carlo Methods in Physics and Chemistry* An Introduction to Quantum Monte Carlo Methods

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 pluriennial 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

*A New Approach to Lattice Gauge Theory* Arcler Press

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.

*Statistical Mechanics: Algorithms and Computations* World Scientific

The technological means now exists for approaching the fundamental limiting 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 molecular-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 large number, not necessarily fixed, of electrons within a charge pulse. The associated reservoirs and sinks of charge carriers may be profitably tapped and manipulated to provide macro-currents which can be readily amplified or curtailed. On the other hand, modern semiconductor ULSI has progressed by adopting a linear scaling principle to the down-sizing of individual semiconductor devices.

**Quantum Monte Carlo Simulations of Ultracold Bosons in a Double Well** Springer Science & Business Media

First published in 2007, this second edition describes the computational methods used in theoretical physics. New sections were added to cover finite element methods and lattice Boltzmann simulation, density functional theory, quantum molecular dynamics, Monte Carlo simulation, and diagonalisation of one-dimensional quantum systems. It covers many different areas of physics research and different computational methodologies, including computational methods such as Monte Carlo and molecular dynamics, various electronic structure methodologies, methods for solving partial differential equations, and lattice gauge theory. Throughout the book the relations between the methods used in different fields of physics are emphasised. Several new programs are described and can be downloaded from [www.cambridge.org/9781107677135](http://www.cambridge.org/9781107677135). The book requires a background in elementary programming, numerical analysis, and field theory, as well as undergraduate knowledge of condensed matter theory and statistical physics. It will be of interest to graduate students and researchers in theoretical, computational and experimental physics.

**Physics and Applications** OUP USA

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.

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*Quantum Monte Carlo Study of Pseudopotentials and Metal Surfaces* Cambridge University Press

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.

*Interface Between Quantum Information and Statistical Physics* Cambridge University Press

The Schrodinger equation is the master equation of quantum chemistry. The founders of quantum mechanics realised how this equation underpins essentially the whole of chemistry. However, they recognised that its exact application was much too complicated to be solvable at the time. More than two generations of researchers were left to work out how to achieve this ambitious goal for molecular systems of ever-increasing size. This book focuses on non-mainstream methods to solve the molecular electronic Schrodinger equation. Each method is based on a set of core ideas and this volume aims to explain these ideas clearly so that they become more accessible. By bringing together these non-standard methods, the book intends to inspire graduate students, postdoctoral researchers and academics to think of novel approaches. Is there a method out there that we have not thought of yet? Can we design a new method that combines the best of all worlds?

*Numerical Quantum Dynamics* Oxford 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.

*An Introduction to Computational Physics* Cambridge University Press

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 advancing 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, 2nd edn. 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 computers or parallel computers, more efficient analysis of simulated systems configurations, and methods to reduce critical slowing down at phase 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.

**Granular Nanoelectronics** World Scientific

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 Schrodinger 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 Schaefer's 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.

**Exploring the Quantum** Springer Science & Business Media

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.

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**Advances in Polaron Physics** John Wiley & Sons

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* Morgan & Claypool Publishers

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.

Springer Science & Business Media

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.

*Electron Correlations and Materials Properties 2* Springer Science & Business Media

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.

*Springer Handbook of Metrology and Testing* Springer Science & Business Media

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 quantum physics and computing. On the other way the topics discussed are not addressed to the specialist. This work bridges hopefully the gap between advanced students, graduates and researchers looking for computational ideas beyond their fence and the specialist working on a special topic. Many important 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 fundamental 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 methodical ansatz useful in all subareas and not necessarily restricted to physics. Of course this methods are related to computational aspects, which means numerical and algebraic methods, but also the interpretation and visualization of huge amounts of data.

*An Introduction to Quantum Monte Carlo Methods* World Scientific

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  $4^{\text{He}}$  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.

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- I had to read this book for school, at the beginning i didn't wanted to read it because it seems so long and boring, when i began to read it i realized that it was an awesome book! the story, the characters, the environment, it was awesome! incredible! sometimes it's hard to understand but some pages after you'll find out what was it all about!!!!!!!you should read it!