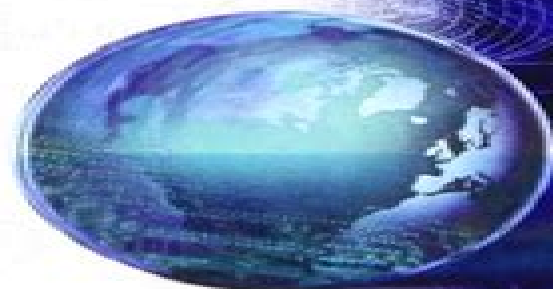


Quantum Monte Carlo Methods in Condensed Matter Physics

Editor

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Quantum Monte Carlo Methods In Condensed Matter Physics

Kurt Binder



Quantum Monte Carlo Methods In Condensed Matter Physics:

Quantum Monte Carlo Methods in Condensed Matter Physics Masuo Suzuki, 1998 Quantum Monte Carlo Methods In Condensed Matter Physics Masuo Suzuki, 1993-12-30 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 T_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.

The Monte Carlo Method in Condensed Matter Physics Kurt Binder, 2012-12-06 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 in Current Physics Vol 7, 1st edn 1979, 2nd edn 1986) and *Applications of the Monte Carlo Method in Statistical Physics* (Topics in Current Physics 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, spin glasses and quadrupolar glasses etc.

Quantum Monte Carlo Methods in Condensed Matter Physics Masuo Suzuki, 1993 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

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Quantum Monte Carlo Approaches for Correlated Systems Federico Becca, Sandro Sorella, 2017-11-30 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

The Monte Carlo Method in Condensed Matter Physics Kurt Binder, 2014-01-15

A Guide to Monte Carlo Simulations in Statistical Physics David P. Landau, Kurt Binder, 2000-08-17 This book describes all aspects of Monte Carlo simulation of complex physical systems encountered in condensed matter physics and statistical mechanics as well as in related fields such as polymer science and lattice gauge theory The authors give a succinct overview of simple sampling methods and develop the importance sampling method In addition they introduce quantum Monte Carlo methods aspects of simulations of growth phenomena and other systems far from equilibrium and the Monte Carlo Renormalization Group approach to critical phenomena The book includes many applications examples and current references and exercises to help the reader

Quantum Monte Carlo Methods James Gubernatis, Naoki Kawashima, Philipp Werner, 2016-06-02 The first textbook to provide a pedagogical examination of the major algorithms used in quantum Monte Carlo simulations

Monte Carlo Simulation in Statistical Physics Kurt

Binder, Dieter W. Heermann, 2013-11-11 When learning very formal material one comes to a stage where one thinks one has understood the material. Confronted with a real-life problem the passivity of this understanding sometimes becomes painfully clear. To be able to solve the problem ideas, methods, etc. need to be ready at hand. They must be mastered, become active knowledge in order to employ them successfully. Starting from this idea the leitmotif or aim of this book has been to close this gap as much as possible. How can this be done? The material presented here was born out of a series of lectures at the Summer School held at Figueira da Foz, Portugal, in 1987. The series of lectures was split into two concurrent parts. In one part the formal material was presented. Since the background of those attending varied widely the presentation of the formal material was kept as pedagogic as possible. In the formal part the general ideas behind the Monte Carlo method were developed. The Monte Carlo method has now found widespread application in many branches of science such as physics, chemistry, and biology. Because of this the scope of the lectures had to be narrowed down. We could not give a complete account and restricted the treatment to the application of the Monte Carlo method to the physics of phase transitions. Here particular emphasis is placed on finite size effects.

Quantum Monte-Carlo Programming Wolfgang Schattke, Ricardo Díez Muiño, 2013-08-30 Quantum Monte Carlo is a large class of computer algorithms that simulate quantum systems to solve many-body systems in order to investigate the electronic structure of many-body systems. This book presents a numeric approach to determine the electronic structure of atoms, molecules, and solids. Because of the simplicity of its theoretical concept, the authors focus on the variational Quantum Monte Carlo (VQMC) scheme. The reader is enabled to proceed from simple examples, such as the hydrogen atom, to advanced ones, such as the Lithium solid. Several intermediate steps cover the Hydrogen molecule, how to deal with a two-electron system, going over to three electrons, and expanding to an arbitrary number of electrons, to finally treat the three-dimensional periodic array of Lithium atoms in a crystal. The examples in the field of VQMC are followed by the subject of diffusion Monte Carlo (DMC), which covers a common example, the harmonic oscillator. The book is unique as it provides both theory and numerical programs. It includes rather practical advice to do what is usually described in a theoretical textbook and presents in more detail the physical understanding of what the manual of a code usually promises as a result. Detailed derivations can be found in the appendix, and the references are chosen with respect to their use for specifying details or getting a deeper understanding. The authors address an introductory readership in condensed-matter physics, computational physics, chemistry, and materials science. As the text is intended to open the reader's view towards various possibilities of choices of computing schemes connected with the method of QMC, it might also become a welcome literature for researchers who would like to know more about QMC methods. The book is accompanied with a collection of programs, routines, and data. To download the codes, please follow http://www.wiley-vch.de/books/sample/3527408517_codes.tar.gz.

An Introduction to Quantum Monte Carlo Methods Tao Pang, 2016-12-07 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

Recent Advances in Quantum Monte Carlo Methods W. A. Lester, Stuart M. Rothstein, Shigenori Tanaka, 1997 This 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'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 Pacificchem meeting in December 2000 but the contributions go beyond what was presented there

Quantum Monte Carlo Methods in Physics and Chemistry M.P. Nightingale, Cyrus J. Umrigar, 1998-12-31 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

Recent Advances in Quantum Monte Carlo Methods W. A. Lester, 1997 The quantum Monte Carlo QMC method is gaining interest as a complement to basis set ab initio methods in cases where high accuracy computation of atomic and molecular properties is desired This volume focuses on recent advances in this area QMC as used here refers to methods that directly solve the Schrödinger equation for example diffusion and Green's function Monte Carlo as well as variational Monte Carlo The latter is an approach to computing atomic and

molecular properties by the Monte Carlo method that has fundamental similarities to basis set methods with the exception that the limitation to one particle basis functions to facilitate integral evaluation is avoided This feature makes possible the consideration of many body wave functions containing explicitly interparticle distances a capability common to all variants of QMC

Modern Theories of Many-Particle Systems in Condensed Matter Physics Daniel C. Cabra, Andreas

Honecker, Pierre Pujol, 2012-01-05 Condensed matter systems where interactions are strong are inherently difficult to analyze theoretically The situation is particularly interesting in low dimensional systems where quantum fluctuations play a crucial role Here the development of non perturbative methods and the study of integrable field theory have facilitated the understanding of the behavior of many quasi one and two dimensional strongly correlated systems In view of the same rapid development that has taken place for both experimental and numerical techniques as well as the emergence of novel testing grounds such as cold atoms or graphene the current understanding of strongly correlated condensed matter systems differs quite considerably from standard textbook presentations The present volume of lecture notes aims to fill this gap in the literature by providing a collection of authoritative tutorial reviews covering such topics as quantum phase transitions of antiferromagnets and cuprate based high temperature superconductors electronic liquid crystal phases graphene physics dynamical mean field theory applied to strongly correlated systems transport through quantum dots quantum information perspectives on many body physics frustrated magnetism statistical mechanics of classical and quantum computational complexity and integrable methods in statistical field theory As both graduate level text and authoritative reference on this topic this book will benefit newcomers and more experienced researchers in this field alike

Ab Initio Molecular

Dynamics Dominik Marx, Jürg Hutter, 2009-04-30 Ab initio molecular dynamics revolutionized the field of realistic computer simulation of complex molecular systems and processes including chemical reactions by unifying molecular dynamics and electronic structure theory This book provides the first coherent presentation of this rapidly growing field covering a vast range of methods and their applications from basic theory to advanced methods This fascinating text for graduate students and researchers contains systematic derivations of various ab initio molecular dynamics techniques to enable readers to understand and assess the merits and drawbacks of commonly used methods It also discusses the special features of the widely used Car Parrinello approach correcting various misconceptions currently found in research literature The book contains pseudo code and program layout for typical plane wave electronic structure codes allowing newcomers to the field to understand commonly used program packages and enabling developers to improve and add new features in their code

Recent Advances in Quantum Monte Carlo Methods W. A. Lester, 2002 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 **Coherent Approaches To Fluctuations - Proceedings Of The Hayashibara Forum '95** Masuo Suzuki, Naoki Kawashima, 1995-12-31 This meeting is devoted to discussing new approaches to critical fluctuation quantum fluctuation and relaxation phenomena The main topics include the study of critical fluctuation using perturbational expansions generalized systematic cluster mean field approximations the CAM possible new systematic approaches to quantum fluctuation including quantum Monte Carlo simulations and coherent approaches to fluctuation and relaxation in complex systems such as spin glasses **Fermion Algorithms - Proceedings Of The Workshop** Frithjof Karsch, Hans J Herrmann, 1991-11-01 Novel Monte Carlo Algorithms for Fermionic Systems are badly needed in high energy and solid state physics At this workshop the newest developments in this direction were presented in particular those concerning multi grid techniques cluster algorithms and massively parallel implementations Molecular Simulation of Fluids Richard J. Sadus, 2023-09-16 Molecular simulation allows researchers unique insight into the structures and interactions at play in fluids Since publication of the first edition of Molecular Simulation of Fluids novel developments in theory algorithms and computer hardware have generated enormous growth in simulation capabilities This 2nd edition has been fully updated and expanded to highlight this recent progress encompassing both Monte Carlo and molecular dynamic techniques and providing details of theory algorithms and both serial and parallel implementations Beginning with a clear introduction and review of theoretical foundations the book goes on to explore intermolecular potentials before discussing the calculation of molecular interactions in more detail Monte Carlo simulation and integrators for molecular dynamics are then discussed further followed by non equilibrium molecular dynamics and molecular simulation of ensembles and phase equilibria The use of object orientation is examined in detail with working examples coded in C Finally practical parallel simulation algorithms are discussed using both MPI and GPUs with the latter coded in CUDA Drawing on the extensive experience of its expert author Molecular Simulation of Fluids Theory Algorithms Object Orientation and Parallel Computing 2nd Edition is a practical accessible guide to this complex topic for all those currently using or interested in using molecular simulation to study fluids Fully updated and revised to reflect advances in the field including new chapters on intermolecular potentials and parallel algorithms Covers the application of both MPI and GPU programming to molecular simulation Covers a wide range of simulation topics using both Monte Carlo and molecular dynamics approaches Provides access to downloadable simulation code including GPU code using CUDA to encourage practice and support learning

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