Density matrix quantum Monte Carlo

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We present a quantum Monte Carlo method capable of sampling the full density matrix of a many-particle system at finite temperature. This allows arbitrary reduced density matrix elements and expectation values of complicated non-local observables to be evaluated easily. The method resembles full configuration interaction quantum Monte Carlo but works in the space of many-particle operators instead of the space of many-particle wave functions. One simulation provides the density matrix at all temperatures simultaneously, from $T = \infty$ to $T = 0$, allowing the temperature dependence of expectation values to be studied. The direct sampling of the density matrix also allows the calculation of some previously inaccessible entanglement measures. We explain the theory underlying the method, describe the algorithm, and introduce an importance-sampling procedure to improve the stochastic efficiency. To demonstrate the potential of our approach, the energy and staggered magnetization of the isotropic antiferromagnetic Heisenberg model on small lattices, the concurrence of one-dimensional spin rings, and the Renyi S_2 entanglement entropy of various sublattices of the 6×6 Heisenberg model are calculated. The nature of the sign problem in the method is also investigated.

I. INTRODUCTION

Quantum Monte Carlo (QMC) methods are well established as vital tools in the study of complex many-body quantum systems, often providing highly accurate results. Projector methods such as diffusion Monte Carlo [1, 2] (DMC) and Green's function Monte Carlo [3, 4] (GFMC) grant access to zero-temperature properties by stochastically applying a projection operator to a starting wave function to obtain a statistical sampling of the ground state. The fixed-node approximation [5–8] allows projector QMC to be applied to systems with sign problems and often produces very good results, but its accuracy depends on the quality of the trial nodal surface and is difficult to assess. Another drawback of projector QMC is that expectation values of quantum mechanical observables that do not commute with the Hamiltonian are difficult to calculate [1, 2, 9, 10].

Finite-temperature QMC methods take a different approach. Path-integral Monte Carlo (PIMC) calculations express the partition function, $Z = \text{Tr}(e^{-\beta \hat{H}})$, as a sum of contributions from paths through Hilbert space [11]. With an appropriate update procedure, the paths can be sampled with the correct probabilities, thus allowing finite-temperature expectation values to be evaluated. The stochastic series expansion (SSE) method [12] has much in common with PIMC. These algorithms also allow access to ground-state properties in principle, but in practice the sign problem is often insurmountable at low temperatures.

The full configuration interaction quantum Monte Carlo (FCIQMC) method recently introduced by Booth, Thom and Alavi [13, 14] is a projector method for studying zero-temperature properties, and, as such, has much in common with DMC and GFMC. However, unlike DMC and GFMC, where the sampling of the ground-state wave function is performed in real space, FCIQMC samples the components of the wave function in a discrete basis. Crucially, no prior knowledge of the nodal structure of the ground-state wave function is required to reach the exact ground state. Rather, the sign problem manifests itself in the large but system-specific population of quantum Monte Carlo walkers required in order for the ground state of the Hamiltonian to emerge [15] from the background noise. The system sizes accessible to FCIQMC are limited by the amount of memory available to store these walkers. However, the method has proven highly successful in many chemical systems, reducing the memory needed to achieve FCI-quality results by several orders of magnitude [16–20]. This has led to much interest in this direction and research into fundamental improvements and new applications of the algorithm continues [17, 21].

This article presents a closely-related QMC method, which we call density matrix quantum Monte Carlo (DMQMC). Like the path-integral and SSE methods, DMQMC allows finite-temperature results to be calculated. However, it uses a projection approach to achieve this and thus has more in common with zero-temperature QMC methods. DMQMC was inspired by FCIQMC and shares many of its features, but samples the elements of the density matrix instead of the components of the wave function in a discrete basis. This enables expectation values of arbitrary quantum mechanical observables to be calculated easily, even when the operator corresponding to the observable does not commute with the Hamiltonian. Such expectation values are difficult to calculate using other QMC methods [1, 2, 9, 10]. Moreover, the ability to directly sample the density matrix means that many quantum information measures are accessible.

[Density Matrix Quantum Monte Carlo Method Spiral Home](#)

James Gubernatis,Naoki Kawashima,Philipp Werner

Density Matrix Quantum Monte Carlo Method Spiral Home:

Quantum Monte Carlo Methods in Physics and Chemistry M.P. Nightingale,Cyrus J. Umrigar,1998-12-31 This book contains lectures on the basic theory and applications of quantum Monte Carlo methods with contributions written by authorities in the field Although tutorial in nature it includes current developments Both continuum systems and lattice models are covered The applications include atomic molecular and solid state physics statistical and low temperature physics and nuclear structure Suitable for Ph D students and beyond **Science Citation Index** ,1992 Vols for 1964 have guides and journal lists *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 **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 Tc 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 **Monte Carlo Methods in Quantum Problems** M.H. Kalos,2012-12-06 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   <u>Novel Applications and Development of the Quantum Monte Carlo Method</u> John Allen White Harkless,2001   **Monte Carlo Methods For Applied Scientists** Ivan Tomov Dimov,2007-12-21 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   *Density Matrix Theory and Applications* Karl Blum,1996-10-31 Quantum mechanics has been mostly concerned with those states of systems that are represented by state vectors In many cases however the system of interest is incompletely determined for example it may have no more than a certain probability of being in the precisely defined dynamical state characterized by a state vector Because of this incomplete knowledge a need for statistical averaging arises in the same sense as in classical physics The density matrix was introduced by J von Neumann in 1927 to describe statistical concepts in quantum mechanics The main virtue of the density matrix is its analytical power in the construction of general formulas and in the proof of general theorems The evaluation of averages and probabilities of the physical quantities characterizing a given system is extremely cumbersome without the use of density matrix techniques The representation of quantum mechanical states by density matrices enables the maximum information available on the system to be expressed in

a compact manner and hence avoids the introduction of unnecessary variables The use of density matrix methods also has the advan tage of providing a uniform treatment of all quantum mechanical states whether they are completely or incompletely known Until recently the use of the density matrix method has been mainly restricted to statistical physics In recent years however the application of the density matrix has been gaining more and more importance in many other fields of physics **Quantum Monte Carlo Methods for First Principles Simulation of Liquid Water** ,2009 *Monte Carlo Methods in Ab Initio Quantum Chemistry* B. L. Hammond,W. A. Lester,Peter James Reynolds,1994 This book presents the basic theory and application of the Monte Carlo method to the electronic structure of atoms and molecules It assumes no previous knowledge of the subject only a knowledge of molecular quantum mechanics at the first year graduate level A working knowledge of traditional ab initio quantum chemistry is helpful but not essential Some distinguishing features of this book are **Recent Advances In Quantum Monte Carlo Methods - Part Ii** William A Lester,Stuart M Rothstein,Shige Tanaka,2002-02-27 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 **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 ad vancing the understanding of various scientific problems Widespread applications of the Monte Carlo method to various fields of the statistical mechanics of condensed matter physics have already been reviewed in two previously published books namely Monte Carlo Methods in Statistical Physics Topics Curro Phys Vol 7 1st edn 1979 2ndedn 1986 and Applications of the Monte Carlo Method in Statistical Physics Topics Curro Phys Vol 36 1st edn 1984 2nd edn 1987 Meanwhile the field has continued its rapid growth and expansion and applications to new fields have appeared that were not treated at all in the above two books e g studies of irreversible growth phenomena cellular automata interfaces and quantum problems on lattices Also new methodic aspects have emerged such as aspects of efficient use of vector com puters or parallel computers more efficient analysis of simulated systems con figurations and methods to reduce critical slowing down at i hase transitions Taken together with the extensive activity in certain traditional areas of research simulation of classical and quantum fluids of macromolecular materials of spin glasses and quadrupolar glasses etc **Quantum Monte Carlo Methods** James Gubernatis,Naoki Kawashima,Philipp Werner,2016-06-02 Featuring detailed explanations of the major algorithms used in quantum Monte Carlo simulations this is the first textbook of its kind to provide a pedagogical overview of the field and its applications The book provides a comprehensive introduction to the Monte Carlo method its use and its foundations and

examines algorithms for the simulation of quantum many body lattice problems at finite and zero temperature These algorithms include continuous time loop and cluster algorithms for quantum spins determinant methods for simulating fermions power methods for computing ground and excited states and the variational Monte Carlo method Also discussed are continuous time algorithms for quantum impurity models and their use within dynamical mean field theory along with algorithms for analytically continuing imaginary time quantum Monte Carlo data The parallelization of Monte Carlo simulations is also addressed This is an essential resource for graduate students teachers and researchers interested in quantum Monte Carlo techniques *Quantum Monte Carlo* James B. Anderson,2007-04-05 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 Recent Advances In Quantum Monte Carlo Methods William A Lester,1997-05-02 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 Schr dinger 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   *Computational Physics: An Introduction To Monte Carlo Simulations Of Matrix Field Theory* Badis Ydri,2017-02-07 This book is divided into two parts In the first part we give an elementary introduction to computational physics consisting of 21 simulations which originated from a formal course of lectures and laboratory simulations delivered since 2010 to physics students at Annaba University The second part is much more advanced and deals with the problem of how to set up working Monte Carlo simulations of matrix field theories which involve finite dimensional matrix regularizations of noncommutative and fuzzy field theories fuzzy spaces and matrix geometry The study of matrix field theory in its own right has also become very important to the proper understanding of all noncommutative fuzzy and matrix phenomena The second part which consists of 9 simulations was delivered informally to doctoral students who were working on various problems in matrix field theory Sample codes as well as sample key solutions are also provided for convenience and completeness   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   Quantum Monte Carlo Methods in Equilibrium and Nonequilibrium Systems Masuo Suzuki,2012-12-06 Speech by Toyosaburo Taniguchi Dr Kubo Chairman Distinguished Guests and Friends I am very happy pleased and honored to be here this evening with so many distinguished guests friends and scholars from within this country and from different parts of the world The Taniguchi Foundation wishes to extend a warm and sincere welcome to the many participants of the Ninth International Symposium on the Theory of Condensed Matter which se ries was inaugurated eight years ago through the strenuous efforts of Dr Ryogo Kubo who is gracing us today with his presence We are deeply indebted to Dr Kubo Dr Suzuki and their associates who havE spent an enormous amount of time and effort to make this particular symposium possible We are convinced that the foundation should not be considered as what makes our symposium

a success The success is entirely due I feel to the continuous efforts of the Organizing Committee and of all those who have lent their support to this program In this sense your words of praise about the symposium if any should be directed to all of them So far I have met in person a total of 62 participants in this Division from 12 countries Argentina Belgium Canada Denmark the Federal Republic of Germany France Ireland Israel Rumania Switzerland the United Kingdom and the United States of America with 133 participants from Japan Those friends I have been privileged to make I shall always treasure

Monte Carlo Method for Solving Inverse Problems of Radiation Transfer V. S. Antyufeev,2014-07-24 No detailed description available for Monte Carlo Method for Solving Inverse Problems of Radiation Transfer   *Quantum Monte Carlo Calculations of Static Dielectric Response* Christopher Bowen,1994

Density Matrix Quantum Monte Carlo Method Spiral Home Book Review: Unveiling the Magic of Language

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Table of Contents Density Matrix Quantum Monte Carlo Method Spiral Home

1. Understanding the eBook Density Matrix Quantum Monte Carlo Method Spiral Home
    - The Rise of Digital Reading Density Matrix Quantum Monte Carlo Method Spiral Home
    - Advantages of eBooks Over Traditional Books
2. Identifying Density Matrix Quantum Monte Carlo Method Spiral Home
    - Exploring Different Genres
    - Considering Fiction vs. Non-Fiction
    - Determining Your Reading Goals
3. Choosing the Right eBook Platform
    - Popular eBook Platforms
    - Features to Look for in an Density Matrix Quantum Monte Carlo Method Spiral Home
    - User-Friendly Interface
4. Exploring eBook Recommendations from Density Matrix Quantum Monte Carlo Method Spiral Home
    - Personalized Recommendations
    - Density Matrix Quantum Monte Carlo Method Spiral Home User Reviews and Ratings
    - Density Matrix Quantum Monte Carlo Method Spiral Home and Bestseller Lists

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