



# Monte Carlo Methods in Quantum Problems

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# Monte Carlo Methods In Quantum Problems

**Federico Becca, Sandro Sorella**



## **Monte Carlo Methods In Quantum Problems:**

**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 been carried out. Such 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 suggests that they may offer a new approach to quantum chemistry, one that is independent of basis and 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 areas: as Particle theorists in particular, K. Wilson have drawn attention to the rich analogy between quantum field theory 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. There is much ferment in the calculation of various one-dimensional problems such as the Hubbard model.

**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.

**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

**Monte Carlo Simulation in Statistical Physics** Kurt Binder, Dieter W. Heermann, 2013-03-14 Monte Carlo Simulation in Statistical Physics deals with the computer simulation of many body systems in condensed matter physics and related fields of physics chemistry and beyond to traffic flows stock market fluctuations etc Using random numbers generated by a computer probability distributions are calculated allowing the estimation of the thermodynamic properties of various systems This book describes the theoretical background to several variants of these Monte Carlo methods and gives a systematic presentation from which newcomers can learn to perform such simulations and to analyze their results This fourth edition has been updated and a new chapter on Monte Carlo simulation of quantum mechanical problems has been added To help students in their work a special web server has been installed to host programs and discussion groups <http://www.cptphys.uni-heidelberg.de> Prof Binder was the winner of the Berni J Alder CECAM Award for Computational Physics 2001

**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

**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 Current Physics Vol 7 1st edn 1979 2nd edn 1986 and Applications of the Monte Carlo Method in Statistical Physics Topics 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 of spin glasses and quadrupolar glasses etc

**Monte Carlo Methods in Quantum Problems** M.H. Kalos, 1984-04-30 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 been

carried out. Such 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 suggests that they may offer a new approach to quantum chemistry, one that is independent of basis and 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 areas. As particle theorists in particular, K. Wilson have drawn attention to the rich analogy between quantum field theory 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. There is much ferment in the calculation of various one dimensional problems such as the Hubbard model.

Applications of the Monte Carlo Method in Statistical Physics K. Binder, 2012-12-06 Monte Carlo computer simulations are now a standard tool in scientific fields such as condensed matter physics including surface physics and applied physics problems, metallurgy, diffusion and segregation etc, chemical physics including studies of solutions, chemical reactions, polymer statistics etc, and field theory. With the increasing ability of this method to deal with quantum mechanical problems such as quantum spin systems or many fermion problems, it will become useful for other questions in the fields of elementary particle and nuclear physics as well. The large number of recent publications dealing either with applications or further development of some aspects of this method is a clear indication that the scientific community has realized the power and versatility of Monte Carlo simulations as well as of related simulation techniques such as molecular dynamics and Langevin dynamics, which are only briefly mentioned in the present book. With the increasing availability of recent very high speed general purpose computers, many problems become tractable which have so far escaped satisfactory treatment due to practical limitations: too small systems had to be chosen or too short averaging times had to be used. While this approach is admittedly rather expensive, two cheaper alternatives have become available: i) array or vector processors specifically suited for wide classes of simulation purposes; ii) special purpose processors which are built for a more specific class of problems or in the extreme case for the simulation of one single model system.

*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

**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

**Monte Carlo Simulation in Statistical Physics** Kurt Binder, Dieter Heermann, 2014-01-15 Methods in Computational Chemistry Stephen Wilson, 2013-11-11 When forty years ago as a student of Charles Coulson in Oxford I began work in theoretical chemistry I was provided with a Brunsviga calculator a small mechanical device with a handle for propulsion metal levers for setting the numbers and a bell that rang to indicate overflow What has since come to be known as computational chemistry was just beginning There followed a long period in which the fundamental theory of the golden age 1925-1935 was extended and refined and in which the dreams of the early practitioners were gradually turned into hard arithmetic reality As a still computing survivor from the early postwar days now enjoying the benefits of unbelievably improved hardware I am glad to contribute a foreword to this series and to have the opportunity of providing a little historical perspective After the Brunsviga came the electromechanical machines of the late 1940s and early 1950s and a great reduction in the burden of calculating molecular wavefunctions We were now happy At least for systems containing a few electrons it was possible to make fully ab initio calculations even though semiempirical models remained indispensable for most molecules of everyday interest The 1950 papers of Hall and of Roothaan represented an important milestone along the road to larger scale non empirical calculations extending the prewar work of Hartree and Fock from many electron atoms to many electron molecules and thus into real chemistry

**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 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

**Monte Carlo Methods** Malvin H. Kalos, Paula A. Whitlock, 2008-10-20 This introduction to Monte Carlo methods seeks to identify and study the unifying elements that underlie their effective application Initial chapters provide a short treatment of the probability and statistics needed as background enabling those without experience in Monte Carlo techniques to apply these ideas to their research The book focuses on two basic themes The first is the importance of random walks as they occur both in natural stochastic systems and in their relationship to integral and differential equations The second theme is that of variance reduction in general and importance sampling in particular as a technique for efficient use of the methods Random walks are introduced with an elementary example in which the modeling of radiation transport arises directly from a schematic probabilistic description of the interaction of radiation with matter Building on this example the relationship between random walks and integral equations is outlined The applicability of these ideas to other problems is shown by a clear and elementary introduction to the solution of the Schrodinger equation by random walks The text includes sample problems that readers can solve by themselves to illustrate the content of each chapter This is the second completely revised and extended edition of the successful monograph which brings the treatment up to date and incorporates the many advances in Monte Carlo techniques and their applications while retaining the original elementary but general approach

*Monte Carlo Methods in Chemical Physics* David M. Ferguson, J. Ilja Siepmann, Donald G. Truhlar, 2009-09-09 In Monte Carlo Methods in Chemical Physics An Introduction to the Monte Carlo Method for Particle Simulations J Ilja Siepmann

Random Number Generators for Parallel Applications Ashok Srinivasan David M Ceperley and Michael Mascagni Between  
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 Lipkowitz, Donald B. Boyd, 2009-09-22 THIS BOOK HAS SIX TUTORIALS AND REVIEWS WRITTEN BY INVITED EXPERTS  
 FIVE CHAPTERS TEACH TOPICS IN QUANTUM MECHANICS AND MOLECULAR SIMULATIONS THE SIXTH CHAPTER  
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 CHEMICAL INFORMATION AND COMPUTER SCIENCE Applications of the Monte Carlo Method in Statistical Physics K.  
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 physics including surface physics and applied physics problems metallurgy diffusion and segregation etc chemical physics  
 including studies of solutions chemical reactions polymer statistics etc and field theory With the increasing ability of this  
 method to deal with quantum mechanical problems such as quantum spin systems or many fermion problems it will become  
 useful for other questions in the fields of elementary particle and nuclear physics as well The large number of recent  
 publications dealing either with applications or further development of some aspects of this method is a clear indication that  
 the scientific community has realized the power and versatility of Monte Carlo simulations as well as of related simulation



techniques such as molecular dynamics and Langevin dynamics which are only briefly mentioned in the present book. With the increasing availability of recent very high speed general purpose computers many problems become tractable which have so far escaped satisfactory treatment due to practical limitations: too small systems had to be chosen or too short averaging times had to be used. While this approach is admittedly rather expensive, two cheaper alternatives have become available: too many array or vector processors specifically suited for wide classes of simulation purposes; or special purpose processors which are built for a more specific class of problems or in the extreme case for the simulation of one single model system.

**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 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.

**Few-Body Problems in Physics '98** Bertrand Desplanques, Konstantin Protasov, Bernard Silvestre-Brac, Jaume Carbonell, 2012-12-06 The sixteenth European Conference on Few Body Problems in Physics has taken place from June 1 to June 6 1998 in Autrans a little village in the mountains close to Grenoble. The Conference follows those organized in Peniscola 1995 Amsterdam 1993 Elba 1991 Uzhgorod 1990. The present one has been organized by a group of physicists working in different fields at the University Joseph Fourier of Grenoble who find in this occasion a good opportunity to join their efforts. The core of the organizing committee was nevertheless located at the Institut des Sciences Nucleaires whose physicists especially in the group of theoretical physics have a long tradition in the domain. The Few Body Conference has a natural tendency to be a theoretical one: the exchange about the methods used in different fields is the common point to most participants. It also has a tendency to be a hadronic physics one: the corresponding physics community perhaps due to the existence of experimental facilities devoted to the study of few body systems is better organized. In preparing the scientific program we largely relied on the advices of the International Advisory Committee while avoiding to follow these trends too closely.

Monte Carlo Methods in Statistical Physics Kurt Binder, 2012-12-06 In the seven years since this volume first appeared there has been an enormous expansion of the range of problems to which Monte Carlo computer simulation methods have been applied. This fact has already led to the addition of a companion volume Applications of the Monte Carlo Method in Statistical Physics Topics in Current Physics Vol 36 edited in 1984 to this book. But the field continues to develop further: rapid progress is being made with respect to the implementation of Monte Carlo algorithms; the construction of special purpose computers dedicated to

execute Monte Carlo programs and new methods to analyze the data generated by these programs. Brief descriptions of these and other developments together with numerous additional references are included in a new chapter Recent Trends in Monte Carlo Simulations which has been written for this second edition. Typographical corrections have been made and fuller references given where appropriate but otherwise the layout and contents of the other chapters are left unchanged. Thus this book together with its companion volume mentioned above gives a fairly complete and up to date review of the field. It is hoped that the reduced price of this paperback edition will make it accessible to a wide range of scientists and students in the fields to which it is relevant: theoretical physics and physical chemistry, condensed matter physics and materials science, computational physics and applied mathematics etc.

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