Preface

Fast computers enable the solution of quantum many-body problems by Monte Carlo methods. As computing power increased dramatically over the years, similarly impressive advances occurred at the level of the algorithms, so that we are now in a position to perform accurate simulations of large systems of interacting quantum spins, Bosons, and (to a lesser extent) Fermions. The purpose of this book is to present and explain the quantum Monte Carlo algorithms being used today to simulate the ground states and thermodynamic equilibrium states of quantum models defined on a lattice. Our intent is not to review all relevant algorithms – there are too many variants to do so comprehensively – but rather to focus on a core set of important algorithms, explaining what they are and how and why they work.

Our focus on lattice models, such as Heisenberg and Hubbard models, has at least two implications. The first is obviously that we are not considering models in the continuum where extensive use of quantum Monte Carlo methods traditionally has focused on producing highly accurate ab initio calculations of the ground states of nuclei, atoms, molecules, and solids. Quantum Monte Carlo algorithms for simulating the ground states of continuum and lattice models, however, are very similar. In fact, the lattice algorithms are in many cases derived from the continuum methods. With fewer degrees of freedom, lattice models are compact and insightful representations of the physics in the continuum.

The second implication is a focus on both zero and finite temperature algorithms.[1] On a lattice, it is natural to study phase transitions. In particular, the recent dramatic advances in quantum Monte Carlo lattice methods for the simulation of quantum spin models were prompted by a need for more efficient and effective ways to study finite-temperature transitions. While quantum Monte Carlo is profitably used to study zero temperature phase transitions (quantum critical phenomena),

[1] Temperature zero is a finite temperature, but common usage separates $T = 0$ (zero temperature) from $T > 0$ (finite temperature) when classifying algorithms. Throughout, we adopt the common usage.

some ground state algorithms have no finite temperature analogs and vice versa. In many respects, the lattice is where the current algorithmic action is.

The book is divided into four parts. The first part is a self-contained, more advanced than average, discussion of the Monte Carlo method, its use, and its foundations. With the basics in place, this part then steps toward the more recent worm and loop/cluster Monte Carlo algorithms for simple classical models, and finally for simple quantum models. Our intent is to be as tutorial as possible and impart a good taste for what quantum Monte Carlo is like. In this introduction, we only briefly mention ground state simulations. The foundations for ground state simulations require less introduction, and we wanted to keep Part I reasonably sized so it can be used as teaching material for a course on computational classical and quantum many-body physics.

Parts II and III present the main quantum Monte Carlo algorithms. Part II discusses finite-temperature methods for quantum spin and Fermion systems. The quantum spin chapter, plus its associated appendices, present a more extensive and sophisticated treatment of the worm and loop/cluster algorithms introduced in Part I. The Fermion chapter details the most important methods for the finite-temperature simulation of lattice Fermion models. Many of the formal techniques developed in this chapter are used in the discussion of the zero temperature Fermion methods in Part III. Besides well-established algorithms for Fermionic lattice models, we also discuss the more recent continuous-time Monte Carlo technique for quantum impurity models. This method is the dynamo driving today's lattice calculations based on the dynamical mean-field approximation, which in turn is being coupled to ab initio calculations of the electronic properties of solids. The chapter on impurity models hence connects the lattice and continuum modeling and simulations of many-electron physics.

Part III discusses the two main zero temperature methods, the variational Monte Carlo and the power method. The power method is a more universal term for what is often called the Green's function Monte Carlo method. Part III also includes a special chapter on the use of the power method for the simulation of Fermion systems. It is in this chapter that the "sign problem" is discussed. This problem is the biggest inhibitor to quantum Monte Carlo reaching its full potential.

The final part does not discuss quantum Monte Carlo algorithms but rather topics that accompany their use. First, we present a widely used method to analytically continue simulation data from imaginary time to real time, so dynamical properties can be extracted from finite-temperature simulations. Finally, we address the parallelization of Monte Carlo simulations. While Monte Carlo calculations per se are naturally parallel (the code, with different random number seeds, can be run on independent processors and the results combined when all calculations have finished), this chapter is about a relatively recent trend, namely, the complexity of

simulations is making the sharing of specific computational tasks among several processors desirable or mandatory, and about what is lying in the future, namely, running even more complex simulations on computers with orders of magnitude more processors.

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To the researchers, students, and teachers using this book: we hope that it helps you appreciate and understand the essence of quantum Monte Carlo algorithms. We also hope that it inspires you to develop even better ways to do quantum simulations. Without doubt, this important research tool has limitations needing mitigation to realize its full potential. Realizing this potential, however, will contribute to our understanding of quantum many-body physics, which in the long run is our attractor to this research area and our motivation to explore and develop new algorithms.

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