Preface

This book originates from the lecture notes of the Ph.D. course on numerical simulations for strongly-correlated systems at the International School for Advanced Studies (S.I.S.S.A.) in Trieste. Even though the backbone of this book has been formed over the last fifteen years, almost all chapters have been completely rewritten, reshaped, or heavily modified in order to improve the clarity of the presentation. In addition, the second part of this book (i.e., Chapters 2, 3, and 4) has been taught during the C.E.C.A.M. Summer School on "Atomistic Simulation Techniques for Material Science, Nanotechnology, and Biophysics", held in Trieste from 2011 to 2016. This school was addressed to graduate and undergraduate students who had little experience in numerical simulations and part of the actual presentation has benefited from their suggestions. The book is envisaged for students and young researches, who do not know much on Monte Carlo methods and want to understand how to implement ground-state algorithms on interacting models. After a first chapter dealing with a bird's-eye review on correlated wave functions that have been used in the past, the second part is intended to give a rather pedagogical introduction to simple probability theory (just the concepts that are necessary for the further developments) and methods for statistical samplings, not only based on Monte Carlo techniques but also including molecular-dynamics approaches. The central part of the book deals with variational and projection Monte Carlo approaches that are well established and widely used to treat lattice models (for both fermions and bosons). Finally, the last part provides an introduction to Monte Carlo methods that have been recently developed for electron systems on the continuum.

Our main motivation to convert the preliminary lecture notes into a structured book is to put in a sequential order all the concepts and machineries that are needed for writing efficient codes based upon variational and projection Monte Carlo techniques. Moreover, a modern textbook describing how to treat wave functions within quantum Monte Carlo algorithms was lacking in the portfolio of books treating

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correlated systems. The methods chosen here are influenced by our own research and do not cover all the numerical approaches that are currently used in the field. For example, we do not discuss the algorithms that have been introduced to deal with impurity models, also employed in dynamical mean-field theory (DMFT), and wave functions that are defined by tensor networks, which, in our opinion, although representing a promising route, they are still in their infancy, especially for what concerns the optimization procedure. Instead, we preferred to focus on a selected number of well established methods that have been developed in the last twenty years and have been demonstrated to be very powerful in the description of several lattice models (e.g., Hubbard, $t-J$, Heisenberg, and many others). Excellent books treating various aspects, which are not considered here, are the ones written by Krauth (2006), Gubernatis et al. (2016), and Martin et al. (2016).

In this book, we have followed the scientific development of one of the authors. In fact, a few years ago, it became important to extend all the knowledge acquired in the construction of variational wave functions on the lattice to realistic simulations and perform direct comparisons with experiments. Here, we have introduced the field starting from lattice models, which is clearly original and quite unconventional; nonetheless, we believe that this approach is pedagogical, as any numerical method is more transparent and clearly defined when first applied to lattice models and then extended to more realistic situations. This way of thinking should be intriguing also for expert coming from electronic systems on the continuum, since a different perspective of a conventional method may clarify and make more transparent the original formulation (e.g., the lattice-regularized diffusion Monte Carlo approach for the standard diffusion Monte Carlo).

In the past two decades, there has been a substantial development in Monte Carlo methods for the optimization of variational wave functions and the definition of stable projection techniques, especially for fermionic models. Even though a final solution of correlated models in more than one spatial dimension is still far away elusive, variational wave functions have been proven to provide very accurate approximations to ground states, when compared to exact diagonalizations on small clusters or in particular regimes where exact solutions are known (e.g., when the sign problem is not present or for particularly designed cases where the ground state can be exactly evaluated). In particular, a deep investigation has been dedicated to frustrated Heisenberg models on various lattices (e.g., on square, triangular, honeycomb, and kagome lattices), to pursue the possibility of stabilizing so-called quantum spin liquids. Here, we would like to mention the case of the Heisenberg model on the kagome lattice, for which a variational wave function, constructed from applying the Gutzwiller projector to a non-correlated fermionic state, suggested the possibility that the ground state can be a spin liquid with Dirac cones in the spinon spectrum (i.e., a gapless spin liquid). This approach competes with

other numerical techniques, like density-matrix renormalization group (DMRG) or its extensions based upon tensor networks. In our opinion, the final understanding of this kind of problem will require both unbiased methods, like DMRG in which the wave function is obtained without any initial guess, and more guided (but more transparent) approaches, like the ones based upon a suitable variational state, whose properties can be estimated by Monte Carlo sampling.

Correlated wave functions (and Monte Carlo methods to assess their physical properties) have been largely employed also in relation to the discovery of high-temperature superconductors. For sure, part of the motivation was given by the success of the Bardeen-Cooper-Schrieffer (BCS) theory for standard (low-temperature) superconductors. However, a crucial contribution in this direction was given by Philip Anderson, who suggested that superconductivity may naturally emerge from doping a resonating-valence bond (RVB) insulator, with a mechanism that does not involve phonons like in the BCS theory. Also in this case, suitably optimized RVB states, constructed from Gutzwiller-projected BCS wave functions, have been shown to give remarkably accurate energies, predicting a uniform RVB superconductivity in hole-doped Hubbard and $t-J$ models. Connected to this issue, we mention that a rather accurate description of a *bona fide* Mott insulator, with preformed Cooper pairs, has been accomplished by a full optimization of the Jastrow factor, which generalizes the Gutzwiller factor to include long-range density-density correlations. Then, within Jastrow-Slater wave functions, it has been possible to describe a continuous metal-insulator transition in the paramagnetic sector of the single-band Hubbard model, similarly to what has been obtained within DMFT.

In recent years, simple generalizations of the previous variational states have been used to study several other models, approaching more realistic models with few (or several) orbitals, disorder, and electron-phonon interactions. In all these cases, the enlarged Hilbert space becomes prohibitive for most of the other numerical methods, while the Monte Carlo sampling is relatively unaffected, allowing us to explore problems that are at the frontier of the present research in solid-state physics.

We would like to remark that very few investigations have been performed in the lattice versions of the quantum Hall effect. Indeed, even though, on the continuum, the Laughlin wave function has been pivotal to describe the fractional case with its exotic properties and several generalizations have been proposed over the years (like the Moore-Read state for the $5/2$ filling factor), very few attempts have been done on the lattice (i.e., for the Hubbard-Hofstadter model). We hope that this book will give motivations to pursue this line of research.

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