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Adolfo Avella
Ferdinando Mancini *Editors*

Strongly Correlated Systems

Numerical Methods

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With 106 Figures

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Preface

This volume "Numerical methods for Strongly Correlated Systems", together with the set "Methods and Techniques for Strongly Correlated Systems" it belongs to, builds upon the long-standing experience we have acquired in organizing the "Trainings Course in the Physics of Strongly Correlated Systems" in Vietri sul Mare (Salerno, Italy) since 1996 and our working scientific experience in the field. Running a school for advanced graduate students and junior post-docs, we realized that this field of condensed matter and solid-state physics was missing adequate textbooks and that the whole Strongly Correlated Systems community would benefit by a systematic exposition of the field. The present volume consists of a series of monographs on the most relevant numerical methods currently used to tackle the hoary problem of correlations. Authors have been selected, consulted major experts in the field, among the most world-wide famous scientists who invented or greatly helped to improve/spread the specific method in the community. Each chapter presents the method in a pedagogical way and contains at least one case-study where the method has proved to give a substantial lap forward in the knowledge and a very rich bibliography. The book is mainly intended for neophytes, who will find in one single volume all pieces of information necessary to choose and start learning a numerical method. Also, more experienced researchers would benefit from this volume as they would gain a deeper understanding of what any single technique can really tell them and what cannot. Accordingly, the accent is more on the ideas behind (origins, pros/cons, perspectives, ...) than on the technical details, which are left to the comprehensive bibliography.

We wish to thank all authors of this volume as they all joined this editorial project with enthusiasm and provided the whole community with what we hope will become a relevant resource for any researcher in the field as comprehensive and extended reference.

Salerno, Italy, March 2013

Adolfo Avella
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Foreword

Elbio Dagotto

Abstract The perspective of the author on the important and rapidly growing role of computational techniques in Theoretical Condensed Matter Physics is provided. A brief summary of each of the chapters of the book is also included in this Foreword.

1 Introduction

In elementary courses on Condensed Matter Physics, students learn that a good description of the electronic properties of simple metals, such as copper or silver, can be obtained via the one-electron approximation. The main assumption of this approximation, which works remarkably well for good metals, is that you can solve the quantum mechanical problem of a particle in a large box, mimicking the crystal, and then simply fill the individual levels with spin-up and spin-down electrons until all the electrons that you wish to have are properly located in states of the box, namely filling levels up to the Fermi energy. Alert students often wonder how this miracle occurs since obviously electrons interact with one another via repulsive Coulombic forces, thus invalidating the one-electron approximation. Elaborated rationalizations are then invoked, based on the Fermi liquid ideas, to justify the neglect of those interactions. But then typically, these students will sooner or later attempt to follow a similar rationale to study other more complex materials, discovering with surprise that this "one electron"

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approximation fails miserably in most cases. A famous example is provided by the copper-oxide high temperature superconductors where naive one-electron estimations would predict the parent compound to be a metal while in reality it is a Mott insulator precisely due to the importance of those repulsive forces among the electrons. Then, in general it is crucial to be able to move beyond "one electron" ideas to properly describe the physics of a wide variety of materials that are both of crucial conceptual relevance and technical importance.

However, properly taking into account the correlations between electrons is much easier said than done. Students also know, from their quantum mechanical classes, how difficult it is to be accurate in problems of atomic physics beyond the hydrogen atom, precisely due to that "pesky" Coulomb repulsion between the electrons. Heroic attempts are being made to address the full quantum mechanical Schrödinger equation of electrons in clusters of atoms via Quantum Monte Carlo (QMC) methods in the continuum, but these techniques are not sufficiently developed to satisfy the vast needs that condensed matter theorists have at present to describe the myriad of interesting novel phenomena that our experimental colleagues almost daily unveil. Then, the most common path is to work with model Hamiltonians. These models are constructed by hand under the assumptions that they must satisfy the known symmetries of the system, they must involve local or quasi local interactions, and in general they have to be "reasonable" such as containing "electron hopping" terms only among atoms at short distances from each other, and involving the proper orbitals for electron tunneling to occur. The construction of these models is typically a fun adventure, but then sooner or later the task of solving the model arises and things rapidly become complicated: if we have trouble studying say light atoms with a few electrons, the problem can only get worse if the number of electrons is of the order of Avogadro's number.

It is fair to say that clever approximations have been developed over the years to study interacting many-body systems. For instance, the BCS theory of superconductivity based on a simple variational state and the assumption that a weak electron–electron attractive interaction arises from the time-retarded interactions with phonons, addresses successfully a complex many-body problem. But in general only a small subset of interesting materials admits such simple descriptions. Moreover, an important motive of present-day Condensed Matter Physics is the "competition" of states in families of compounds with rich phase diagrams. These states can be reached in the laboratory by adding or removing electrons, increasing pressures, turning on and off electric or magnetic fields, etc. Having a single "pen and pencil" formalism that allows the study of competing, say insulating and metallic states, is very difficult, particularly if we aim to reach an accurate description of both states. Dealing with complex many-body problems can indeed be frustrating.

Fortunately, the fast development of computers in recent times allows for some hope. How about solving the quantum mechanical many-body problems, with all the important interactions incorporated, using the help of computers? Computers can manipulate large arrays of numbers in tiny amounts of time, way beyond what any human can hope to do in a lifetime. In fact, we are witnessing the slow

evolution of the traditional theoretical physics mainly based on pen and pencil calculations unto a more sophisticated enterprise that often involves large-scale computer simulations. While older generations carved their intuition based on integrals over momentums and frequencies, new generations often think in real space and time and learn to visualize intuitively the physics under discussion from the analysis of complex plots of data arising from the study of model Hamiltonians using elaborated computational techniques. In fact, in my lifetime I have seen the rise of computational physics from an early "supporting actor" role to a much more fundamental role in the study of models and materials. Nowadays nobody blinks when a publication is almost entirely based on results coming from computational efforts. Hopefully, the new generations will appreciate that this did not happen overnight, and will thank in their hearts the pioneers that established computational physics as a well respected, and currently rapidly growing, area of theoretical physics.

In this book, edited by Professors Adolfo Avella and Ferdinando Mancini, the state of the art of computational methods to study model Hamiltonians is presented. This volume is actually one component of a set of three books on the general area of "Strongly Correlated Systems: Methods and Techniques," all of them edited by Avella and Mancini. The first volume, already published recently by Springer, has the title "Theoretical Methods for Strongly Correlated Systems," and the focus is on analytical studies of correlated electrons. A personal observation here about the title of this first book: note that computational physics is a rapidly growing subset of theoretical physics. Thus, describing analytical methods as "theoretical" and computational methods as a separate entity often called "numerical" is incorrect. Both analytical and numerical methods are different methods used to address theoretical physics. The second book in this series is the one you have in your hand now. The third will address "Experimental Techniques for Strongly Correlated Systems." Having a global view of correlated electrons, via its analytical and computational theoretical perspectives and also the experimental component will be very beneficial to young scientists entering into this field.

Returning to the Foreword for this book, note that having powerful computational techniques to carry out the numerical investigations is crucial, because although my casual writing above ("let the computers do the work") may imply that this is relatively easy, in practice it is certainly not. To start with, most of the computational studies are carried out using finite small systems, with the hope of performing a systematic study of many sizes and then an extrapolation to the bulk limit. For this reason, accurate and powerful methods are needed that can handle large clusters. Moreover, sometimes there are subtleties, such as the effect known as the "sign problem" that is widely discussed in several chapters of this book. This effect can certainly spoil the fun of a project. Thus, it is important to be aware of the sort of techniques that are available in the literature for the handling of a particular problem of interest to the reader. Let me make this point clear: there is no single computational technique at present that can handle any problem of your choice, but each method presented in the many chapters of this book has a limited

range of applicability. Young theoretical physicists reading this text should become familiar with all of the methods presented here, and particularly remember the type of problems that each technique is good for.

In the rest of this foreword, I will present a brief description of each of the many chapters of this book (following the order in which they appear), aiming to summarize the essence of each method. But, of course, readers should use my writing only as a stepping stone into the real important portion of the book that are the individual chapters. I will also resist the temptation of citing literature in this foreword, so that readers will have to consult the many chapters to gather that important information.

2 Lanczos Exact Solution of Small Clusters

In Chap. 1, Prelovšek and Bonča describe the Lanczos method, often casually referred to as Exact Diagonalization, both at zero and finite temperature. The essence of this technique is to solve exactly a small cluster of the model Hamiltonian that is under study. While the exponential growth of Hilbert spaces often limits the applicability of this technique to very small systems, the reason for its popularity is that it can be applied to all the families of models that are frequently used in the correlated electron context, although with a cluster size that shrinks fast with the number of degrees of freedom per site. In these regards the technique is flexible and moreover it is truly unbiased: the exact properties of the model in the small cluster used will be obtained as an answer, as opposed to a crude approximation to those properties. Typically, after a Lanczos analysis unveils a particular tendency to spin, charge, or orbital order at the short distances that fit into the small cluster that was solved exactly, then other computational techniques or mean-field approximations can be employed to address larger systems. Reciprocally, the Lanczos method can also be used to confirm ideas, such as proposed variational states, or to gather numerical information to be used as benchmark to judge the accuracy of other computational methods. Lanczos has the important advantage over other algorithms in that it can also be used to gather dynamical information, both in the form of spectral functions or as real-time evolutions of states, the latter including studies far from equilibrium.

Prelovšek and Bonča also describe in Chap. 1 variations of the Lanczos technique, such as the High Temperature expansion method where a reduced set of randomly chosen states are used, as in Monte Carlo procedures. The calculations are carried out for all temperatures simultaneously. Applications of this finite-temperature Lanczos method include the study of the famous two-dimensional t-J model for Cu-oxide high temperature superconductors, addressing subtle issues such as the presence of non-Fermi liquid behavior, the exotic linear resistivities unveiled at optimal hole doping in the cuprates, the existence of pseudogap regions in the underdoped regime, and others. Also, recent variations of the Lanczos technique are presented in this chapter, such as the "low temperature" and

"microcanonical" Lanczos methods, and even the use of a reduced or truncated basis set, illustrated with the example of adding phonons, which is in the spirit of the Density Matrix Renormalization Group (DMRG) technique described in the subsequent chapters of this book.

3 Density Matrix Renormalization Group, Matrix Product States, and the Multi-scale Entanglement Renormalization Ansatz

To improve on the severe size limitations of the Exact Diagonalization or Lanczos method, the DMRG technique was developed by S. White, and four chapters of this book are devoted to this technique (three of them being reviewed here in this subsection simultaneously), including recent variations and improvements. In Chap. 2, Feiguin introduces the reader to the DMRG method by first explaining the fast growth of Hilbert spaces with the number of spins using the spin-1/2 Heisenberg model as illustration. This example clearly shows that to study large systems, a clever basis truncation procedure is needed. In the early days, the Renormalization Group method of K. Wilson was used to construct an approximate basis and the technique worked nicely in several cases. But consider for instance the simple problem of just one electron hopping between nearest-neighbor sites along a chain of length L with open boundary conditions, and suppose we wish to get a good approximation to its ground state by knowing the properties of a chain of length $L/2$. The ground state wave function of the $L/2$ chain has the shape of a cosine function, with nodes at both ends of the chain. If we naively assume that the ground state for the case of length L can be approximated by gluing the two ground states of length $L/2$, then we are generating a spurious node at the center, since we know that the ground state of L only has nodes at the extremes of the chain. Then, the energy alone cannot be the best indicator for how to select a proper truncated basis. As Feiguin explains, it is much better to use the reduced density matrix to select that reduced basis since in this quantity the connection between the two portions of the problem, and their potential quantum mechanical entanglement, is included. Based on these ideas the DMRG method emerges and certainly this technique is the method of choice for quasi one-dimensional electronic model Hamiltonians.

Feiguin explains also the limitations of the DMRG method. For instance, in the early days it was common practice to use the "infinite" system variation of DMRG, but nowadays it is known that addressing finite systems and then extrapolating to the bulk is the best way to go. And of course, carefully analyzing how the results change with the number of states m is a must, since sometimes the behavior of observables with increasing m is not smooth, due to occasional "tunneling" into regions of the Hilbert space that were not included for a smaller m. Another limitation is the generalization to two-dimensional systems: in fact if

we order the sites of a finite ladder or truly two-dimensional lattice via a "snake" procedure to reduce it to a one-dimensional arrangement, it is clear that in the 1D language the hopping terms and interactions, that are not on-site, will develop a long-range character that always complicates any algorithm. Fortunately, considerable progress is being made via the concept of entanglement entropy that allows to understand why the DMRG number of states m that is needed in 2D grows very fast with the number of sites (following an "area law", see also Chap. 3 by Schollwöck). The entanglement entropy is an important concept that establishes that two systems A and B are disentangled when the wave function of the system is merely the product of the wave functions of the individual components, while they are maximally entangled when the state of A uniquely establishes the state of B and vice versa. DMRG in fact minimizes the loss of information related with the entanglement of the components.

The DMRG-related novel area based on the "Matrix Product States" (MPS) is presented in detail by Schollwöck in Chap. 3 (this topic is also mentioned in Chap. 2 by Feiguin). Starting with the mathematical discussion of the main ideas, an example based on the Heisenberg model helps in clarifying the formalism. The MPS perspective establishes DMRG as a variational method in the space of matrix product states, allowing for extensions of the method and a deeper conceptual understanding. The connection between the MPS perspective and the original DMRG algorithm is explained in this chapter. Overall, it is clear that although the novel approaches are not yet in practice better than the original DMRG, surprises may be found in the near future as research in this active field continues progressing based on the MPS perspective.

In Chap. 4, Evenbly and Vidal describe the notion of "tensor network states" as variational states to characterize lattice quantum many-body systems. The number of parameters in this case is much smaller than the exponentially large dimension of the Hilbert space with increasing lattice size. These tensor network states can be classified based on the physical geometry of the system or via the holographic geometry, where an additional dimension parameterizing different lengths or energy scales is introduced. The focus of Chap. 4 is on the latter, in particular on the Multi-scale Entanglement Renormalization Ansatz (MERA) to study critical systems in one-dimensional geometries, aiming to properly capture the scale invariance of these systems. The authors describe in detail all the properties of the MERA method and compare with other techniques, and they also explain how to deal with symmetries. In addition, benchmark results are provided using the critical Ising model and other critical systems, and comparison with results of other methods are discussed. The conclusion of these comparisons is that the MERA method indeed produces better correlators at large distances for critical systems, as the method was originally designed to achieve.

4 Time-Dependent DMRG

In Chap. 5, Feiguin explains the time-dependent DMRG method (this topic was also discussed in Chap. 3 by Schollwöck). This technique allows for the study of real-time dynamics (i.e. not imaginary time but real) and it can provide spectral functions with frequency dependence and also results far from equilibrium. Feiguin explains that as time grows adapting (i.e. changing) the basis is crucial, because the "truncated" or optimal basis for the ground state is not necessarily the same basis that is needed for the state during the time evolution. For instance, this becomes clear for the case of strong perturbations that will drive the system away from the equilibrium state that existed before the perturbation was turned on. In this case, other areas of the Hilbert space may become relevant as, for example, occurs when a steady current develops due to a strong electric field. Thus, it is important to keep track of the entire time-evolution of the wave function: in fact, the propagation of the wave functions becomes the main purpose of the algorithm.

Feiguin explains that the Suzuki–Trotter approach is a natural procedure to break the time evolution operator. It introduces a discretization, i.e., a "Trotter error" that is under reasonable control in practice since this error can always be reduced by reducing the time-step length, of course at the cost of increasing the computer time of the study. In addition, the advantages of the Runge–Kutta integration for these types of methods are discussed in this chapter via concrete examples. Moreover, a similar evolution but in imaginary time can be used to obtain results at finite temperatures, showing the formal similarities with the real-time evolution.

The time-dependent DMRG technique is widely applied these days to problems that range from transport through quantum dots to non-equilibrium physics in the context of cold atoms. In the former, the introduction of a sudden bias to generate a current is often employed, and a plateau in the current versus time is formed in a finite window of time (due to the open boundary conditions, eventually the current will bounce back). Thus, the I–V curve can be studied for those quasi-stationary currents. Several other time-dependent correlation functions can be calculated as well. Feiguin also describes the "enemies" of these methods: they are related with the entanglement entropy, and with the abrupt versus adiabatic introduction of modifications in the Hamiltonian. For instance, to study the effects of a strong perturbation it may be advantageous to turn on this perturbation "slowly" so that the system has time to select the proper basis to describe the new system.

5 Loop Algorithm

In Chap. 6, Todo explains how a quantum model can be mapped into a classical model by adding another dimension related with temperature, which is then discretized in steps. This is equivalent to working in imaginary time. Moreover, Todo

also explains that there is a continuous-time path-integral representation that can be alternatively used. The world-line configurations are introduced for the stochastic sampling, involving products of matrix elements, and it is emphasized that millions of spins can be handled by this procedure. However, note that these matrix elements can be negative, thus leading to "sign problems" which of course introduces a limitation in the type of models that can be handled with these technique. While this is a complication difficult to avoid, Todo discusses that another typical problem of Monte Carlo simulations, the slowing down of the simulations at low temperatures or near criticality, can actually be improved upon or eliminated altogether via cluster algorithms where groups of spins are simultaneously flipped, instead of using individual spins for the updates. This reduces critical slowing down near continuous phase transitions, particularly if the cluster sizes are chosen based on the correlation lengths of the problem. Another procedure to avoid the lack of ergodicity addresses global constraints in the simulation, via a generalization of phase space. In this case auxiliary variables are introduced that represent constraints in the spin system, to fight conservation rules that make the single site update procedure useless. For instance, if the total spin S_z must be conserved, the flip of a spin will always be rejected. For this reason, procedures involving bonds as opposed to single sites are sometimes more natural. Thus, the ability of the programmer is needed to identify the correct variables to use to carry out the simulations in an efficient manner. In the case of the spin-1/2 antiferromgnetic Heisenberg chain, introducing the imaginary time direction leads to a representation in terms of loops that thus becomes an integral part in the updating process.

6 Stochastic Series Expansion

In Chap. 7, Melko discusses the Stochastic Series Expansion (SSE) technique, which is a very efficient QMC method for quantum lattice models. This technique was originally devised by A. Sandvik as a finite-temperature simulation based on a Taylor expansion of the partition function. The method is easy to implement and applies to quantum spins and bosons, as long as they do not have the "sign problem." As simple examples, Melko discusses the spin-1/2 isotropic Heisenberg model and the Ising model in a transverse field. In general a quantum D dimensional problem must be mapped into a $D + 1$ dimensional classical representation incorporating an imaginary time axis to allow for its implementation in classical computers. In the SSE method the trace of products of the Hamiltonian are evaluated stochastically, formally via path integral or world-line representations. Cluster and loop algorithms are used to speedup the simulation and allow for ergodicity. More recently, the method has been reformulated to become applicable to the zero-temperature projector method, where a large power of the Hamiltonian is applied to a trial wavefunction to project out the ground state. Both methods are in principle conceptually quite different, but their implementation via non-local

loop or cluster algorithms reveals an underlying similarity, as discussed by Melko via the example of the Heisenberg model in a valence bond basis.

7 Quantum and Variational Monte Carlo

In Chap. 8, Sorella discusses the very powerful QMC technique and the associated Variational Monte Carlo (VMC) method. For model Hamiltonians and in regions of parameter space where QMC "works", namely where there are no "sign problems" or other technical inconveniences, the QMC method is very powerful and addresses exactly (within statistical errors) the physics of the model under investigation. Sorella explains that the somewhat tedious process of gathering statistics to reduce error bars can be easily parallelized by running different realizations of the Monte Carlo evolution at different nodes of a computer cluster. For instance, after arriving to an equilibrium configuration, at each node a different "random number set" can be used to continue the runs with that configuration as a start. The results of the many Monte Carlo time evolutions at those different nodes can be eventually gathered at the end of the runs to construct averages. Considering that there are supercomputers with $\sim 100,000$ nodes these days, clearly this procedure is advantageous since its scalability adapts to the number of nodes available. Of course we must be aware of the complications that arise in QMC and similar algorithms when we are near criticality since in these cases the self-correlation time diverges (namely the number of Monte Carlo steps needed to generate statistically independent equilibrium configurations diverges at second order transitions). And of course we must worry about sign problems, as explained before. But where it works, QMC is indeed very powerful and unbiased.

With regard to the VMC method, the relation with QMC arises from the need to calculate the expectation values in the variational state via a Monte Carlo stochastic process. Definitely starting with a "good" wave function is a must for accuracy, and Sorella uses the case of the Gutzwiller wave function to illustrate how a simple projector operator that removes doubly occupied sites can make an important difference for the case of the famous (or infamous depending on your view) Hubbard model. Dealing with many-body variational wave functions often illuminates the physics under discussion, thus VMC tends to provide qualitative insight into the problem studied even if it is not as precise and unbiased as QMC is. Since the Nobel prizes for the BCS theory of superconductivity and the Fractional Quantum Hall effect were essentially given for proposing an excellent (and simple) multi-electronic variational wave function, it is clear that variational approaches have some appeal. These days VMC can be carried out with a very large number of free parameters to optimize, and moreover, there are proposed methods to systematically improve a starting wave function.

8 Coupled Cluster Technique for Quantum Chemistry and Nuclear Physics

In Chap. 9, Kowalski et al. describe the coupled cluster (CC) formalism. This is a widely employed and accurate method for the solution of the Schrödinger equation in molecules and other intrinsically finite systems. For instance, the technique is mainly applied in the context of computational chemistry but it is also used in nuclear physics. Correlation many-body effects are properly captured by the CC formalism, contrary to perturbative methods. These correlation effects are crucial to understand molecular structures, chemical reactions, and bond-forming/bond-breaking processes.

The CC method starts with an exponential Ansatz involving the exponential of the cluster operator T acting over a single Slater determinant, such as the one arising from the Hartree-Fock approximation. T is a sum over the many-body components. The authors explain that including higher order excitations in the process comes at a high numerical price, leading to severe limitations of the straightforward procedure even for relatively small systems. But the authors also explain that there are several interesting improvements to deal with this problem, including the use of leadership class computer architectures. Often the cases of the H_2O and CO_2 molecules are used as examples to judge the accuracy of the results, and in some tests, up to 210,000 cores of supercomputers have been used. Extensions to the always complex case where there are quasi-degenerate states are also presented by the authors. In the rest of the chapter, the several variations of the methodology are reviewed in considerable detail. It is concluded that at present accurate calculations can be carried out for 200–300 correlated electrons with 1,300–1,500 basis set functions.

9 Monte Carlo Methods for Diagrammatic Series

Chapter 10 by Prokof'ev reviews the basic principles of the Diagrammatic Monte Carlo (DiagMC) and Worm Algorithm techniques. With regard to DiagMC, the simpler case that comes to mind are the Feynman diagrams as they appear in standard perturbative formulations of Quantum Electrodynamics, or in similar diagrammatic formulations of problems of Condensed Matter Physics. The DiagMC method discussed in this chapter is generic and simply aims towards an accurate estimation of a sum of multiple integrals. However, Prokof'ev clarifies that DiagMC is fundamentally different from simply listing all diagrams of order say less than a maximum number, and then evaluating via Monte Carlo each integral one by one. In fact, in DiagMC the order of the diagram, their topology, and internal and external variables are all treated on equal footing, and each diagram represents a "point" in a generalized configuration space. A unique feature of DiagMC is that instead of addressing finite systems with increasing size

as in most computational techniques described in this book, the technique applies directly to the Feynman diagram series. Thus, results are obtained already in the thermodynamic limit and at any temperature.

Prokof'ev addresses the "sign blessing" issue (as opposed to the "sign problem" issue widely discussed in other chapters): due to the fact that the Feynman diagrams can be positive or negative, the apparent fast growth of the number of diagrams with their order, and the associated impression that the series are just asymptotic, is removed by the sign alternation. In fact, it is thanks to the sign blessing in this context that the series do converge.

With regard to the Worm Algorithm, this technique allows for a better sampling of configuration space in cases where this space has a complex topology and/or global constraints, which usually induce complications in standard Monte Carlo methods based on local updates, since the Monte Carlo time evolution leads to nominal equilibrium states that are actually trapped in a portion of the configuration space. In this case, there are ergodicity problems since not all sectors of configuration space are equally sampled. In practice, the method is based on enlarging the original configuration space with the original constraints into a larger space without those constraints. This facilitates the "tunneling" between different sectors. Examples dealing with the Ising, XY, and bosonic models are discussed in this chapter.

10 Continuous Time Quantum Monte Carlo

In Chap. 11, Gull and Troyer provide an introduction to "continuous time quantum Monte Carlo" (CT-QMC) methods for fermions. The description includes both lattice models, such as the Hubbard model, and quantum impurity problems, such as the Anderson impurity problem describing a magnetic atom embedded in a non-interacting medium. Impurity problems formally appear also in the solution of the Dynamical Mean Field Theory (DMFT) equations, and it is in this area where CT-QMC methods are used the most frequently at present. CT-QMC is based on the stochastic sampling of time-dependent diagrammatic perturbation theory, as described by Prokof'ev in Chap. 10. Time is continuous from the beginning, since there is no need to discretize this dimension, contrary to what is done in many other techniques presented in this book. Gull and Troyer explain that at present there are already several types of extensions of this method (called hybridization, interaction, and auxiliary method) with different areas of applicability. These three variations are explained in detail in the bulk of the chapter. The authors include an introduction to the general diagrammatic Monte Carlo formulation, with sums involving not only the order of the diagrams but also their topology in order for ergodicity to be satisfied (see Chap. 10 by Prokof'ev). The issue of the sign problem is also discussed, and it is concluded that in impurity problems, this complication is not as severe as in finite-sized lattice models.

In the second half of the chapter, the authors provide several examples that illustrate the wide range of applicability of the continuous-time methods. The examples include Kondo problems and quantum dots, single-site and cluster DMFT, the three-dimensional Hubbard model above the critical temperature for antiferromagnetism, LDA + DMFT approaches to real materials, and even real-time dynamical methods.

11 Summary

In this Foreword, my goal has been to transmit to the readers my profound enthusiasm for the field of research centered at the computational studies of model Hamiltonians. With just a few exceptions, it is difficult to find analytical techniques that are reliable for the study of a particular model in the area of Strongly Correlated Electrons since usually there is no small parameter to use in an expansion. Thus, after applying those techniques we always have the uneasy feeling of not really knowing if the results are accurate. However, with the use of computational methods, calculations can have a much more robust foundation. Employing the computer for the study of a model has the feeling of an experiment: you can ask clever "questions" to the "sample" under study, analyze data, and come up with an intuitive picture of what is happening. Very often the computer results are not what we were expecting a priori, thus there is a neat back and forth process until a convergence to a firm conclusion is reached. The many chapters in this book illustrate on how sophisticated the computational methods have become in recent years, with plenty of interesting new tricks and perspectives being developed and applied to address challenging issues in the study of a variety of model Hamiltonians. And in the meantime, while we work hard on these types of problems, the computer industry is constantly improving the machines that we use in our effort! For all these reasons, I am convinced that this area of research has a promising future and hopefully it will continue to attract outstanding researchers such as the many authors of the chapters contained in this book.

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Chapter 1
Ground State and Finite Temperature Lanczos Methods

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Abstract The present review will focus on recent development of exact-diagonalization (ED) methods that use Lanczos algorithm to transform large sparse matrices onto the tridiagonal form. We begin with a review of basic principles of the Lanczos method for computing ground-state static as well as dynamical properties. Next, generalization to finite-temperatures in the form of well established finite-temperature Lanczos method is described. The latter allows for the evaluation of temperatures $T > 0$ static and dynamic quantities within various correlated models. Several extensions and modification of the latter method introduced more recently are analysed. In particular, the low-temperature Lanczos method and the micro-canonical Lanczos method, especially applicable within the high-T regime. In order to overcome the problems of exponentially growing Hilbert spaces that prevent ED calculations on larger lattices, different approaches based on Lanczos diagonalization within the reduced basis have been developed. In this context, recently developed method based on ED within a limited functional space is reviewed. Finally, we briefly discuss the real-time evolution of correlated systems far from equilibrium, which can be simulated using the ED and Lanczos-based methods, as well as approaches based on the diagonalization in a reduced basis.

1.1 Introduction

Models of strongly correlated systems have been one of the most intensively studied theoretical subjects in the last two decades, stimulated at first by the discovery of compounds superconducting at high-temperatures and ever since by the emergence

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of various novel materials and phenomena which could be traced back to strongly correlated electrons in these systems. Recently, cold atoms in optical lattice offer a different realization of strongly correlated quantum entities, whereby these systems can be even tuned closer to theoretical models.

One of the most straightforward methods to numerically deal with the lattice (discrete) models of correlated particles, which are inherently many-body (MB) quantum systems, is exact diagonalization (ED) of small-size systems. In view of the absence of well-controlled analytical methods, ED method has been employed intensively to obtain results for static and dynamical properties of various models with different aims: (a) to search and confirm novel phenomena specific for strongly correlated systems, (b) to test theoretical ideas and analytical results, (c) to get reference results for more advanced numerical techniques.

MB quantum lattice models of interacting particles are characterized with a dimension of the Hilbert space given by the number of basis states $N_{st} \propto K^N$ that is in turn exponentially increasing with the lattice size N, where K is the number of local quantum states. It is therefore clear that ED methods can treat fully only systems with limited N_{st}, i.e., both K and N must be quite modest.

Among the ED approaches the full ED within the Hilbert space of the model Hamiltonian, yielding all eigenenergies and eigenfunctions, is the simplest to understand, most transparent and easy to implement. In principle it allows the evaluation of any ground state (g.s.) property as well as finite temperature $T > 0$ static or dynamic quantity, at the expense of very restricted N_{st}. In spite of that, it represents a very instructive approach but also remains essentially the only practical method when all exact levels are needed, e.g., for studies of level statistics.

Lanczos-based ED methods have already long history of applications since Cornelius Lanczos [1] proposed the diagonalization of sparse matrices using the iterative procedure, allowing for much bigger Hilbert spaces N_{st} relative to full ED. Lanczos diagonalization technique is at present a part of standard numerical linear algebra procedures [2, 3] and as such in solid state physics mainly used to obtain the g.s. energies and wavefunction with corresponding expectation values. The approach has been quite early on extended to calculation of the dynamical response functions within the g.s. [4]. The method has been in the last 20 years extensively used in connection with models related to high-T_c materials, for which we can refer to an earlier overview [5].

The present review will focus on recent development of ED-based and Lanczos-based methods. The basics of the Lanczos method are presented in Sect. 1.2 and its application for g.s. properties in Sect. 1.3. One of already established generalizations is the finite-temperature Lanczos method (FTLM) [6, 7], reviewed in Sect. 1.4, which allows for the evaluation of $T > 0$ static and dynamic properties within simplest models. Several extensions and modifications of the latter have been introduced more recently, in particular the low-temperature Lanczos method (LTLM) [8] and the microcanonical Lanczos method (MCLM) [9], particularly applicable within the high-T regime.

Since the application of the ED methods there have been attempts and proposals for the proper choice of reduced basis which could allow for the study of bigger systems. While this is clearly very broad subject with most substantial

achievements in one-dimensional (1D) systems within the framework of the density-matrix renormalization-group (DMRG) idea, there are also successful applications in higher D $>$ 1 combined with the Lanczos procedure being reviewed in Sect. 1.5. Recently, there is also quite an intensive activity on studies of real-time evolution of correlated systems, both under the equilibrium and the non-equilibrium conditions that can be simulated using the ED and Lanczos-based methods, as discussed in Sect. 1.6.

1.2 Exact Diagonalization and Lanczos Method

1.2.1 Models, Geometries and System Sizes

ED-based methods are mostly restricted to simple models with only few local quantum states K per lattice site in order to reach reasonable system sizes N. Consequently, there are only few classes of MB models that so far exhaust the majority of ED and Lanczos-method studies, clearly also motivated and influenced by the challenging physics and relevance to novel materials and related experiments.

To get some feeling for available sizes reachable within the ED-based approaches, it should be reminded that in full ED routines the CPU time scales with the number of operations $Op \propto N_{st}^3$, while the memory requirement is related to the storage of the whole Hamiltonian matrix and all eigenvectors, i.e., $Mem \propto N_{st}^2$. This limits at present stage of computer facilities the full ED method to $N_{st} < 2 \cdot 10^4$ MB states. On the other hand, using the Lanczos-based iterative methods for the diagonalization of sparse matrices (Hamiltonians), CPU and memory requirements scale as $Op, Mem \propto N_{st}$, at least in their basic application, to calculate the g.s. and its wavefunction. In present-day applications this allows the consideration of much larger basis sets, i.e., $N_{st} < 10^9$. Still, lattice sizes N reached using the Lanczos technique remain rather modest, compared to some other numerical approaches as the DMRG and quantum-Monte-Carlo (QMC) methods, if the full Hilbert basis space relevant for the model is used.

The simplest nontrivial class of MB lattice models are spin models, the prototype being the anisotropic Heisenberg model for coupled $S = 1/2$ spins,

$$H = \sum_{\langle ij\rangle\alpha} J_{ij}^{\alpha\alpha} S_i^{\alpha} S_j^{\alpha}, \tag{1.1}$$

where the sum $\langle ij\rangle$ runs over pairs of lattice sites with an arbitrary interaction $J_{ij}^{\alpha\alpha}$ (being in principle anisotropic) and S_i^{α} are component of local $S = 1/2$ operator. The model has $K = 2$ quantum states per lattice site and therefore allows for biggest N in the ED-based approaches where $N_{st} \propto 2^N$ basis states. To reduce N_{st} as many symmetries and good quantum numbers as practically possible are used to decompose the Hamiltonian into separate blocks. Evident choice are sectors with