Exotic phases of matter in quantum magnets

A tensor networks tale

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CHAPTER 1

Introduction

1.1 Interacting many-body systems

As a rule of thumb, physical systems that are made up of a large number of constituent particles—also known as *many-body systems*—become more complicated as the interactions between the particles become stronger. When there are no interactions present, a system is called *free* or *non-interacting*. Free systems are relatively easy to understand because they are effectively one-particle systems, and there are many examples of one-particle systems that are analytically solvable. Since no real particle is actually free, one might be tempted to conclude that free systems are solely of theoretical interest. However, there exists a plethora of real physical systems that are very well approximated by a free theory. For example, dilute Alkali gases at low temperatures have a scattering length that is much smaller than all other length scales relevant for the gas (such as the average distance between the atoms and the thermal de Broglie wavelength), and are therefore practically free[1], which allows them to Bose-condense; see [6] and references therein. Another common example is that of electrons in semiconductors and in most metals; in accordance with Fermi-liquid theory [7], due to the screening effect of the positively charged lattice ions, these electrons can be effectively described as free particles with a renormalized mass that is different from the actual electron mass.

It is quite remarkable that Fermi-liquid theory provides an accurate description of electrons in a metal, because the electrons themselves are far from free: they

[1] With the exception of an effective Dirac-delta inter-atomic interaction that makes the Alkali atoms behave like hard-core bosons.

strongly repel each other through their mutual Coulomb repulsion. Since the particles in the free theory are not the actual particles that make up the system—the mutually strongly repelling electrons—Fermi-liquid theory provides what is known as a *quasiparticle* description of electrons in a metal. It should be noted that quasiparticles do not need to be directly related to the actual particles that constitute the system at hand. For example, vibrations in a lattice can be described in terms of phonons, quasiparticles that represent collective vibrational modes of the lattice [8]. The fact that quasiparticles can be very different from the original particles that make up a given system, is an example of what Anderson famously argued in his 1972 article 'More is different' [9], namely: that the effective description of the system in question cannot necessarily be completely deduced from the underlying microscopic system, and, continuing along this line of thought, that every science is fundamental in its own respect.

When the (quasi)particles describing a system are weakly interacting, the system can be studied by means of *perturbation theory*: which amounts to starting from non-interacting particles, and then successively adding corrections such that the sum of those corrections on top of the free theory converges to the original interacting theory. Perturbation theory is a very powerful method of investigation; it has been applied successfully in a surfeit of different contexts, ranging from planetary orbitals [10] to Feynman diagrams used in quantum field theories [11].

1.2 Strongly correlated materials

It can of course happen that there is no known free system that resembles the system of interest. Examples of such systems are *strongly correlated materials*, which are characterized by the property that their dynamical particles are not known to be (approximately) describable in terms of non-interacting (quasi)particles. Strongly correlated materials are inherently difficult to study.

The strong inter-particle interactions present in strongly correlated materials allow for the underlying quantum mechanics that governs the constituent particles to manifest itself on macroscopic length scales. As such, strongly correlated materials often have unusual—possibly technologically interesting—electronic and magnetic properties. For this reason, a substantial part of condensed matter physics concerns itself with finding methods that provide better insight into this interesting class of materials.

A well-known example of quantum mechanics manifesting itself at every-day length scales is that of superconductivity: a phenomenon that describes materials that below a certain critical temperature exhibit zero electrical resistance and expel magnetic fields from their interior. Whereas conventional superconductors can be understood in terms of the condensation of Cooper pairs—known as Bardeen-Cooper-Schrieffer (BCS) theory [12], the mechanism behind high temperature su-

perconductivity to this day remains to be understood. The two main hypothesis for explaining high temperature superconductivity are: (1) that neighboring electrons form valence bonds [13, 14], which in the presence of doping combine into a resonating valence bond (RVB) state, and (2) that the electron paring is mediated through short-range spin waves (see [15] and references therein).

Another topic of interest within the field of strongly correlated materials is topological order, which arises when there exist several degenerate ground states with differing patterns of long-range entanglement that cannot change into each other without going through a phase transition [16]. Topological order is different from conventional order, in that the former cannot be understood within the Ginzburg-Landau paradigm [17] of spontaneous symmetry breaking. Systems that exhibit topological order have properties that are promising for future technological applications, such as excitations that obey fractional [18, 19] (even non-abelian [20, 21]) statistics that are interesting for quantum computing [22], and topologically protected edge states [23] that could potentially be used for electronic devices. In addition, related to the above there is also the phenomenon of *deconfined criticality* [24], which involves an emergent gauge field and deconfined degrees of freedom at the critical point separating two quantum phases.

The theoretical models underlying the above-mentioned phenomena involve systems that consist of electrons that hop around on a lattice formed by the ions that make up the solid in question. Of these models, the Hubbard model [25, 26] is the one that has been studied most intensely over the years. Originally, the Hubbard model was proposed independently by Gutzwiller [27], Kanamori [28] and Hubbard [25] in 1963 as a simplified model for electrons in solids. It is based on the tight binding approximation, in which electrons occupy atomic orbitals and electrical conduction is represented by electrons hopping from one site to the next—mathematically expressed by nearest-neighbor hopping terms in the Hamiltonian with coupling parameter $-t$. The only interaction terms present are on-site repulsive interactions—representing the Coulomb repulsion between nearby electrons—that increase the energy of the system by U whenever a site is doubly occupied, making the Hubbard model one of the simplest models of interacting particles on a lattice. The challenging parameter regime is when U and t are of comparable magnitude, and there is no natural small parameter in which to express perturbative series. It is precisely in this regime for which it is expected that the Hubbard model is relevant for high temperature superconductivity in cuprates.

Theoretical models—such as the Hubbard model—that are obtained by stripping the underlying microscopic model of all its characteristics but the most essential ones, are known as *effective models*. The main idea behind such a simplification is that, if done correctly, the model in question retains all the essential features of the original material that is being modeled, yet is simple enough to be studied theoretically. Because of their apparent simplicity, effective models like the Hub-

bard model often serve as archetypes for the type of order they display, and are interesting to study in their own right because of what they can teach us about how quantum many-body systems behave. Despite their simplicity, however, they can be notoriously hard to tackle. The Hubbard model, for example, has only been solved exactly in one dimension [29].

1.3 Quantum magnets

At half filling[2], and in the limit of strong on-site repulsion $U \gg t$, each spin particle is fixed to a lattice site and the Hubbard model becomes an insulator. Neighboring spin particles gain kinetic energy by anti-aligning [30], resulting in an effective nearest-neighbor interaction called the *exchange interaction* [31]—also known as the *Heisenberg interaction* [32]. The effective model arising from the strongly repulsive Hubbard model at half filling is called the *Heisenberg model*[3].

Lattice models with a spinful particle pinned to each lattice site are called *quantum magnets*. Well-known quantum magnets are the quantum Ising model: the quantum version of the classical Ising model proposed by Wilhelm Lenz to his then doctoral student Ernst Ising in an effort to obtain microscopic understanding of the phenomenon of ferromagnetism [33], and the above-mentioned Heisenberg model.

Due to their quantum mechanical nature, quantum magnets can offer surprisingly rich physics. Especially in the presence of competing interactions or geometric frustration [34]—which occurs when, at the level of product states, the ground state does not minimize the energy on all bonds simultaneously—ground states of quantum magnets can display exotic types of order that go beyond ordinary ferro and antiferromagnetism. An example of this is the above-mentioned RVB state—introduced by Anderson in 1973 [13] as a proposed ground state of the geometrically frustrated triangular lattice antiferromagnet[4]—also known as a *spin liquid*. While preserving spin-rotation and lattice rotation and translation symmetries, spin liquids can instead display *non-local* order [37, 38]. In addition, quantum magnets can exhibit many other interesting types of order, such as such as *spin-nematic* order that involves the breaking of spin-rotational symmetry while preserving time-reversal symmetry [39].

The main objects of study of this thesis are all two-dimensional quantum magnets that fall within the category of either the bilinear-biquadratic Heisenberg or the Shastry-Sutherland type models.

[2] Meaning that there is exactly one particle per site.

[3] The exchange interaction can cause nearby spin particles to either anti-align (super exchange), or align (direct exchange). Usually, the super exchange interaction is an order of magnitude larger than the direct exchange interaction [30].

[4] It was later shown numerically that the triangular lattice antiferromagnet has a ground state that displays 120° magnetic ordering instead [35, 36].

Because of their strong inter-particle interactions, investigating quantum magnets is challenging, and exact solutions are difficult to be found in dimensions higher than one. Consequently, physicists are forced to resort to numerical methods, and this is the approach that we shall take in the chapters to come.

1.4 Numerical many-body physics

One of the main difficulties with simulating quantum many-body systems lies in the fact that the Hilbert space $\mathcal{H}$ describing the total system is a tensor product[5] of all single-particle Hilbert spaces $\mathcal{H}_i$:

$$\mathcal{H} = \bigotimes_{i=1}^{N} \mathcal{H}_i,$$

where N is the total number of particles. Throughout this thesis, in agreement with the quantum magnets to be investigated, all single-particle Hilbert spaces are taken to be finite dimensional, with the same[6] dimension d. Assuming the latter, the dimension of the total Hilbert space $\mathcal{H}$ scales exponentially in the number of particles,

$$\dim H = d^N.$$

As a consequence, directly simulating real systems—which contain of the order of Avogadro's number $6.022 \cdot 10^{23}$ of particles—even with an optimistic extrapolation of Moore's law [40] is out of the question on classical computers in the foreseeable future. The exponential scaling of the Hilbert space becomes particularly problematic when approaching the thermodynamic limit $N \to \infty$, which is technically required in order to investigate quantum phase transitions. To deal with this obstacle, physicists have developed all kind of methods to tackle interacting many-body systems.

Exact diagonalization of the Hamiltonian by means of Lancoz's method [41] is possible for systems of up to about fifty particles (see, e.g. Ref. [42]), which is far from the thermodynamic limit. However, smart extrapolations to infinite sizes can in principle be done using finite-size scaling, and therefore exact diagonalization is a useful method when there is not a lot of prior information available about the many-body system under investigation.

As a method that is insensitive to the exponential scaling of the Hilbert space, quantum Monte Carlo (QMC) [43]—being based on statistical sampling—offers a very powerful and popular approach to tackle many-body systems. QMC has the advantage that it is very well controlled, and given enough computation time any

[5] Modulo some action of a permutation group if the particles are indistinguishable.
[6] Since all particles pinned to the lattice sites have the same total spin $S = \frac{d-1}{2}$.

desired accuracy can be reached. The main trick of QMC is to map a quantum system to a classical probabilistic system—in the spirit of Feynman's path integral—to which ordinary Monte Carlo can be applied. The problem is, that this trick in general does not work for either geometrically frustrated or fermionic systems, because of the appearance of negative probabilities. The occurrence of these negative probabilities is known as the *sign problem* [44]. As a consequence, there is a large set of strongly correlated systems that is as of yet beyond the reach of QMC. *The systems that we shall investigate fall into this category for those parts of the parameter regimes that we are interested in.*

There is also a variety of approximate methods. To name a few: mean field theory works well for higher dimensional systems [45], but for lower dimensional systems—especially those that are strongly correlated—it typically fails to capture the quantum correlations; series expansion techniques [46] rely on perturbation theory, which requires a small parameter to expand in; and spin wave theory [47] can be very useful, but it is biased because it requires a classical ground state to start from and can therefore overlook quantum ground states that do not have a classical analogue.

To summarize, each of the approaches described above has its own shortcomings, and developing appropriate methods to investigate strongly correlated quantum many-body systems that suffer from the sign problem is one of the major challenges of contemporary condensed matter physics.

For this thesis, we shall take a different approach to dealing with the immense size of the N-body Hilbert space: that of *tensor networks*. The main idea behind the application of tensor networks to quantum mechanics is to *not* consider the total Hilbert space as a whole, but instead focus on a smaller subset of the Hilbert space that only scales linearly in the system size N, and is therefore much more manageable numerically. Compared to the other methods mentioned above, tensor network algorithms are unbiased, not restricted to a particular type of systems, and in addition have the added advantage that they can also work directly in the thermodynamic limit, making them a very powerful tool for investigating strongly correlated many-body systems. Needless to say, tensor networks also have their limitations, and we shall discuss those in detail in Chapter 2.

1.5 Ground state phase diagrams

Obtaining full understanding of a quantum mechanical system requires—in principle—to overcome the immensely daunting task of diagonalizing its Hamiltonian, or computing its partition function. Unless the system has enough symmetries to make it exactly solvable (by for example Bethe-ansatz like methods [48]), or there exists an efficient way to statistically sample the system along the lines of QMC, obtaining complete knowledge of the system at hand is extremely diffi-

cult. Instead, we will undertake a first step towards understanding the system by computing its ground state(s). Knowing the ground state gives insight into the system considered, not only because it is important to understanding the low energy properties of the system, but also because it provides a basis upon which excited states can be constructed.

In the presence of competing interactions, by continuously varying coupling constants in the Hamiltonian, the ground state of a given system can display different types of order. If a change in order happens abruptly, meaning that the ground state energy changes non-analytically, we speak of a *quantum phase transition*. Quantum phase transitions carry the label *quantum* because, contrary to classical phase transitions, the former occur at zero rather than finite temperature, and are governed by quantum effects.

Phase transitions are interesting objects of study by themselves. Whereas first order transitions typically signify an abrupt jump from one phase to the next, (conventional) continuous second order transitions exhibit *universal* behavior, expressed in terms of *scaling relations* [49–51] between critical exponents that describe how certain properties diverge when approaching the transition point. The scaling relations can be understood in terms of Wilson's renormalization group [52, 53]; they are universal in the sense that they are insensitive to the microscopic details of the system. However, the more interesting phase transitions are those that go beyond the Ginzburg-Landau framework, such as those mentioned in Sections 1.2 and 1.3.

For each model investigated in this thesis, we shall compute its ground states and determine the nature of the transitions that separate them, all of which will be summarized in the *ground state phase diagram* of the model in question.

1.6 Outline

This thesis concerns itself with models that fall within two types of two-dimensional quantum magnets: the nearest-neighbor spin-1 *bilinear-biquadratic Heisenberg* (BBH)-type models and the *Shastry-Sutherland* (SSL)-type models. Several models of either type will be investigated by means of tensor network algorithms, and accurate descriptions of their ground state phase diagrams will be provided.

Chapter 2 motivates the use of tensor networks, especially for the simulation of ground states. In particular, the infinite-system tensor network known as iPEPS, which stands for *infinite projected entangled pair state*, will be discussed, and notable attention will be given to the main bottleneck in dealing with infinite two-dimensional tensor network states: that of contracting infinite networks. Furthermore, ample detail will be given on the optimization algorithms used to obtain approximate ground states with iPEPS, which include both imaginary-time-evolution and variational-update based optimizations.

Chapter 3 discusses the spin-1 BBH model, a model that is not only of experimental relevance because it contains the SU(3)-Heisenberg model that can be realized using cold atoms, but is also theoretically interesting because it is the most general spin-rotation, lattice-rotation and lattice-translation symmetric spin-1 model with only nearest-neighbor interactions. Chapter 3 focuses on the square-lattice version of the spin-1 BBH model, which is home to two different nematic phases that break on-site spin-rotation symmetry through anisotropies in their spin fluctuations. More interestingly, our iPEPS study will show that there are two additional phases that were not known to be present on the square lattice BBH model: a partially magnetic partially nematic phase, and a quantum paramagnetic phase, the latter of which can be adiabatically connected to the famous Haldane phase of decoupled one-dimensional spin-1 BBH spin chains.

Chapter 4 continues the investigation of Chapter 3 by studying the spin-1 BBH model on the numerically more challenging and experimentally more relevant triangular lattice. Indeed, the triangular magnets $NiGa_2S_4$ and $Ba_3NiSb_2O_9$ have been shown to exhibit spin-liquid-like behavior, and partial explanations that have been proposed for this behavior involve the nematic ground states of the triangular lattice spin-1 BBH model. Motivated by the discovery of the partially magnetic partially nematic and quantum paramagnetic phases on the square lattice, an in-depth investigation of both the isotropic and the anisotropic triangular lattice BBH model will be provided. Surprisingly, neither of the above-mentioned additional phases shows up in the ground state phase diagram on the triangular lattice BBH model.

Chapter 5 investigates the SSL model, which is known to admit an exact ground state made up of a product of singlet dimers. By varying the coupling parameters, the SSL model interpolates between this dimer ground state and the Néel-ordered ground state of the square lattice Heisenberg antiferromagnet. The long standing debate on what happens at the interplay of the dimer and antiferromagnetic phases, which seemed to have converged on the existence of the intermediate so-called *empty plaquette phase*, was reinvigorated by a recent experimental paper by Zayet et al. [54] that claimed that the ground states in between the dimer and AFM phases lie in the *full* rather than the empty plaquette phase. In order to get to the bottom of these contradictory statements, by simulating both plaquette phases using iPEPS, we will demonstrate that the ground state indeed lies in the aforementioned empty plaquette phase. Moreover, our simulations will show that the ground state remains in the empty plaquette phase even in the presence of a small artificial bias in the Hamiltonian towards the full plaquette phase.

Chapter 6 focuses on the sign problem within quantum Monte Carlo—the method of choice for unfrustrated quantum magnets—and examines it within the context of the *extended SSL model* equipped with additional inter-dimer couplings that continuously interpolate between the original SSL and the fully-frustrated bilayer Heisenberg model. We will demonstrate that that the sign problem disappears for

some values of the coupling parameters. By comparing to our iPEPS study of the ground state of this extended SSL model, the region for which the sign problem disappears will be shown to be completely contained within the dimer phase. This phenomenon can be understood in terms of an artificial sign-free Hamiltonian that shares its ground state with the extended SSL model for part of its coupling parameter regime. As a consequence, thermodynamic properties can potentially be accurately modeled by quantum Monte Carlo even for frustrated quantum magnets provided that the ground is shared with another sign-free Hamiltonian.

Finally, in **Chapter 7**, we will summarize all findings presented in the following chapters, put them into a broader perspective, and provide an outlook for possible future research projects that continue the work set out in this thesis.