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Exotic Phases of Matter in Quantum Magnets

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Summary

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A Tensor Networks Tale

In many-body systems, the complex interplay between the particles that make up the system can lead to unexpected collective behavior, giving rise to *exotic phases of matter*. Well-known examples of such exotic phases are superfluids, which describe flow with zero viscosity; superconductors, which have zero electrical resistance and expel magnetic fields from within; and spin liquids: quantum many-body states that remain disordered down to zero temperature and can display topological order. Usually, these exotic phases involve the emergence of quantum mechanical effects at macroscopic length scales, which typically occurs in strongly correlated systems.

This thesis focuses on a subcategory of strongly correlated systems: insulating solids for which the dynamical particles—the electrons—are pinned to a background lattice, and the remaining degrees of freedom are their quantum mechanical spins. Such systems are called *quantum magnets*. Their constituent particles typically interact with Heisenberg-type interactions. Despite being described by relatively simple Hamiltonians, quantum magnets can exhibit very interesting physics, ranging from ordinary ferro and antiferromagnetism to nematic order and spin-liquid-like behavior.

The strong inter-particle interactions present in strongly correlated systems, and quantum magnets in particular, make them difficult to study, and force physicists to resort to numerical methods—especially for models of dimension higher than one. Due to the exponential scaling of the Hilbert space in the number of particles, however, brute-force numerical computations are doomed to fail for systems that consist of anywhere near the number of particles that real systems are made up of. Therefore, smart algorithms that allow for simulation of *large* strongly correlated systems are in great demand.

Based on statistical sampling, thus insensitive to the size of the many-body Hilbert space, quantum Monte Carlo (QMC) is one of the physicists' principal lines of at-

tack. However, it turns out that a large class of strongly correlated systems—such as fermionic and frustrated systems—suffer from the *sign problem*, which makes QMC inviable. One of the main challenges of contemporary numerical many-body physics is to either come up with ingenious ways to circumvent the sign problem, or invent alternative methods.

This is where *tensor networks* come in. A many-body quantum state, which itself is one gigantic tensor, can be decomposed into a network made up of contractions of smaller local tensors. These local tensors carry a parameter, called the *bond dimension*, which determines how much entanglement can be captured by the tensor network state in question. Rather than performing numerical simulations on the entire Hilbert space, the simulations can be restricted to the much more manageable subset of fixed-bond-dimension tensor network states. If the needed level of accuracy requires it, the bond dimension can afterwards be extrapolated to infinity to obtain results that, in principle, are exact.

In this thesis several interesting quantum magnets are investigated by means of tensor networks. Specifically, we use *infinite projected entangled pair states* (iPEPS) to study two-dimensional quantum magnets directly in the thermodynamic limit; a necessary limit for the investigation of quantum phase transitions that separate different quantum phases.

Chapter 3 discusses the spin-1 bilinear-biquadratic Heisenberg (BBH) model on the square lattice. The BBH model is interesting experimentally because it contains the SU(3) Heisenberg model that can be realized using cold atoms. Moreover, being the most general lattice-translation, lattice-rotation and spin-rotation symmetric spin-1 system with nearest-neighbor interactions, the BBH Hamiltonian is also interesting from a theoretical point of view. Besides the known magnetic and nematic phases, our tensor network study of the square lattice BBH model demonstrates the occurrence of two additional phases that had been overlooked by previous studies: a partially magnetic partially nematic phase, and a paramagnetic phase that preserves spin-rotation and lattice-translation symmetries but breaks lattice-rotation symmetry. By studying the anisotropic square lattice BBH model, we continue to show that this paramagnetic phase can be adiabatically connected to the well-known Haldane phase of decoupled spin-1 chains.

Motivated by the unusual and not-well-understood behavior of the triangular lattice quantum magnets $NiGa_2S_4$ and $Ba_3NiSb_2O_9$, we then proceed to investigate the triangular lattice BBH model in Chapter 4. Our iPEPS simulations reproduce both the ferroquadrupolar and antiferroquadrupolar phases that were suggested to be realized in $NiGa_2S_4$. Interestingly, both the partially magnetic partially nematic phase as well as the extended Haldane phase found on the square lattice turn out to be absent from the triangular lattice phase diagram. However, our study does show that the triangular lattice BBH model is susceptible to lattice distortions, and that even in the absence of the biquadratic coupling, the system on the triangular lattice undergoes a transition to the Haldane phase at about

80% anisotropy.

Chapter 5 focuses on a different quantum magnet, the *Shastry-Sutherland* (SSL) model. This model has been studied extensively because (i) it is one of the few two-dimensional magnets for which an exact eigenstate—made up of a product dimer singlets—is known, and (ii) it is realized experimentally in $SrCu_2(BO_3)_2$. The dimer eigenstate is actually the ground state of the SSL model for weak inter-dimer coupling. For strong inter-dimer coupling, the ground state is a Néel ordered square lattice antiferromagnet (AFM). There has been ongoing debate on what happens in between the dimer and AFM phases, but most works agree that there exists an intermediate plaquette phase. However, the nature of the plaquette phase has been questioned by a recent experimental paper that examined $SrCu_2(BO_3)_2$ under external pressure, and argued in favor of the so-called *full plaquette phase*; this in contrast to the conclusion stated in other recent theoretical papers that claim that the *empty* rather than the full plaquette phase occurs in between the dimer and AFM phases. By directly comparing the energies of both plaquette states, we show that the intermediate phase is the empty plaquette phase. However, a bias in the Hamiltonian towards the full plaquette phase of only a few percent makes the full plaquette state the lowest energy state, which shows that the SSL model is susceptible to anisotropies. It is not unlikely that subjecting $SrCu_2(BO_3)_2$ to external pressure distorts the lattice non-uniformly, making the full plaquette state energetically favorable over the empty plaquette one.

Finally, Chapter 6 examines an extension of the SSL model (which interpolates between the ordinary SSL and the fully-frustrated bilayer models) in the context of the sign problem in QMC. It turns out that, when expressed in the dimer basis, the sign disappears at low temperatures. This has to do with the fact that the dimer ground state of the SSL model is also the ground state of an artificial sign free model obtained by making all off-diagonal elements of the Hamiltonian non-positive (in the dimer basis). A comparison with our iPEPS study shows that, as expected, the regime wherein the sign problem disappears is contained within the dimer phase of the extended SSL model. Using QMC, the magnetic susceptibility and specific heat are computed for the SSL model. The above demonstrates that knowledge of an exact ground state can possibly be used to accurately compute thermodynamic quantities of frustrated systems by means of QMC.