Exotic phases of matter in quantum magnets

A tensor networks tale

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CHAPTER 7

Conclusion

In this thesis, we have investigated the intricate ground state physics of several two-dimensional quantum magnets of spin-1 bilinear-biquadratic Heisenberg (BBH) and Shastry-Sutherland (SSL) type. Making use of infinite projected entangled pair states (iPEPS), introduced in Chapter 2, we were able to study the models of interest directly in the thermodynamic limit.

In the BBH model on the square lattice, discussed in Chapter 3, we encountered two additional phases that had not been found in previous studies: a partially magnetic partially nematic phase in between the antiferroquadrupolar and ferromagnetic phases, and a quantum paramagnetic phase separating the antiferromagnetic and 120° magnetically ordered phases. Interestingly, the anisotropic square lattice BBH model taught us that the intermediate quantum paramagnetic phase is adiabatically connected to the Haldane phase of decoupled one-dimensional spin-1 BBH chains. Our finding of these two additional phases reaffirms the strength of iPEPS as an ansatz for simulating two-dimensional strongly correlated systems.

Inspired by our discoveries on the square lattice, in Chapter 4 we turned our attention to the experimentally more relevant triangular lattice BBH model. Our iPEPS study reproduced the nematic phases proposed to provide an effective description of the not-fully-understood quantum magnet $NiGa_2S_4$. Remarkably, neither of the two additional phases found on the square lattice manifest themselves on the triangular lattice; nor did we find any other signs of paramagnetic phases. However, our study of the *anisotropic* triangular lattice did teach us that the Haldane phase occupies a large portion of the phase diagram of the anisotropic model, reaching up to about a value of $J_{\text{anis}} \approx 0.8$ around the Heisenberg point $\theta = 0$ where the biquadratic terms is absent. The observation that the Haldane phase extends further at the Heisenberg point on the anisotropic triangular lattice than it does on the anisotropic square lattice, reflects the fact that, due to frustration, the 120° magnetically ordered state on the triangular lattice is less stable than the Néel ordered antiferromagnetic state on the square lattice. Perhaps this insight could be used to attempt to realize the two-dimensional Haldane phase in a triangular lattice antiferromagnet subjected to external pressure.

A question that comes to mind is whether a Haldane phase occurs in spin-1 BBH models on different lattices. Because the triangular lattice has a larger coordination number than the square lattice, it is tempting to hypothesize that the Haldane phase is unlikely to occur for densely connected lattices. Intuitively, this makes sense, because the energy gained by forming valence bonds in one particular direction at the cost of increasing the energy of the remaining bonds seems beneficial only when there are not too many remaining bonds. For lattices with a small coordination number on the other hand, if a possibility exists to form short valence bond loops—which is the case on the honeycomb [67] and Kagome [244] lattices—the ground state will break translational symmetry by forming short loops (of length six and three respectively). Moreover, a very recent study of the star-shaped lattice by Lee and Kawashima [177] showed that a spin-liquid-like phase appears in a region that encompasses the parameter regime wherein we found the Haldane phase on the square lattice. The spin-liquid-like states have lower bond energies on the triangles that make up the lattice [245], and we suspect that also here the state forms short valence bond loops (around the triangles). Only on the square lattice the system prefers infinitely long Haldane chains over short (four-site) valence bond loops.

Motivated by the study by Zayed et al. [54] that examined $SrCu_2(BO_3)_2$ by exposing it to varying external pressure, in Chapter 5 we focused on a different quantum magnet: the Shastry-Sutherland model that effectively describes the magnetic properties of $SrCu_2(BO_3)_2$. Zayed et al. suggested that the phase separating the dimer and antiferromagnetic phases of the SSL model is the *full* plaquette phase, thereby contradicting a fair amount of studies that instead argued in favor of the *empty* plaquette phase. From our iPEPS study of the SSL model, we learned that, in agreement with the latter, the empty plaquette state is lower in energy. However, the full plaquette state becomes energetically favorable when we apply an artificial bias on the full plaquettes of only a few percent. The discrepancy between Zayed et al.'s and the other above-mentioned works actually makes sense in the context of our result if we assume that the pressure applied to $SrCu_2(BO_3)_2$ distorts the lattice non-uniformly, in such a way that not all effective inter-dimer couplings change by an equal amount.

Interestingly, the effects of pressure on $SrCu_2(BO_3)_2$ have been investigated theoretically by the work of Moliner et al. [213], wherein the authors argued that a lattice distortion due to external pressure could give rise to yet another emergent Haldane phase. Remarkably then, the distorted spin-1/2 SSL model is effectively described by an anisotropic square lattice spin-1 model that lies in the same ground state phase as the spin-1 square lattice BBH model discussed earlier. As a topic of future study, it would be interesting to investigate if and how this Haldane phase of the distorted SSL model is related to the full plaquette phase of the biased SSL model.

In Chapter 6, we took a different turn, and investigated the sign problem that arises in quantum Monte Carlo (QMC) in the context of an extended Shastry-Sutherland model that interpolates between the original SSL and the fully-frustrated bilayer models. We showed that, because the dimer ground state of the SSL model is also the ground state of an artifical sign-free Hamiltonian, the extended SSL model can actually in part be investigated by QMC at low temperatures. Using iPEPS, we determined that the region wherein the sign problem disappears is, however, completely contained within the dimer phase. If the sign-free region would have encompassed also a part of the plaquette phase, rather than relying on exact diagonalization of small systems as done by Zayed et al., QMC could possibly have been used to obtain a more accurate description of the relationship between external pressure applied to $SrCu_2(BO_3)_2$ on the one hand, and the coupling parameters in the SSL model on the other. Regardless, the observation that the sign problem disappears when the ground state is shared with a sign-free Hamiltonian could possibly be used to study thermodynamic properties by means of QMC of several other frustrated systems for which an exact ground state is known.

Having tackled various challenging quantum magnets, we can conclude that tensor networks, and iPEPS in particular, are very capable of uncovering the complex inner workings of strongly correlated materials. Further development of these algorithms will hopefully galvanize the discovery of other unexpected phenomena and also provide a better understanding of the collective behavior of the inherently quantum mechanical many-body systems that make up the world around us.