Quantum Spin Liquids in SU(N) Heisenberg Models: Variational Monte Carlo Study of Dynamical Correlations

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In two and three dimensions, the SU(2) Heisenberg model usually has magnetically ordered (ferromagnetic or antiferromagnetic) ground states. In these cases, the excited states are typically bosonic spin 1 magnons. However, if quantum fluctuations are sufficiently enhanced—whether through geometric frustration or by expanding the local Hilbert space—the antiferromagnetic Heisenberg model can develop a disordered ground state, known as a quantum spin liquid. Under such conditions, the bosonic spin 1 magnons are split into two fermionic spin 1/2 quasiparticles (spinons). The splitting of the bosonic excitation to a pair of fermionic quasiparticles is called fractionalization. Consequently, the existence of the quantum spin liquid ground state and the fractionalized excitations is directly measurable through the dynamical spin structure factor $S(\mathbf{k},\omega)$, if at the lowest excitation energies we observe a continuum (implicating a pair of quasiparticles) instead of a single branch.

In my PhD, I calculated the $S(\mathbf{k},\omega)$ of the antiferromagnetic SU(N) Heisenberg model in the fundamental representation on different lattices, assuming gapless quantum spin liquid ground states. To do so, I applied a numerical variational Monte Carlo method (VMC) introduced for the study of the antiferromagnetic SU(2) Heisenberg model. In this method, the ground state is approximated by a Gutzwiller-projected Fermi sea obtained from mean-field theory, and the excited states are constructed in the subspace of Gutzwiller-projected particle-hole excitations of the Fermi sea.

To validate the VMC method on an exactly solvable SU(N) symmetric model, I computed the $S(\mathbf{k},\omega)$ of the SU(3) Heisenberg chain. I showed that the low energy spectrum and the distribution of the spectral weights of the SU(3) Heisenberg chain can be well reproduced by this method, by comparing the $S(\mathbf{k},\omega)$ to exact diagonalization results for 18 sites, the two-soliton continuum of the Bethe Ansatz, DMRG results and conformal field theory for 72 sites [1].

I computed the $S(\mathbf{k},\omega)$ of the SU(4) Heisenberg model on the honeycomb lattice, approximating the ground state by the Gutziller projected π-flux Fermi sea, called a Dirac spin liquid (DSL). I compared these results with non-interacting mean-field calculations. The two approaches produce qualitatively similar results, suggesting that the energy spectrum of the Gutzwiller projected excitations may also be a gapless continuum of fractionalized excitations. Quantitatively, the Gutzwiller projection shifts the spectral weight to lower energies, thus emphasizing the lower edge of the continuum [2].

I proposed the Gutzwiller projected π-flux Fermi sea (another DSL) as the ground state of the SU(6) Heisenberg model on the Kagome lattice. I investigated the energetical stability of the DSL against perturbations of the mean-field ansatz and confirmed that the DSL remained the lowest energy singlet state. Furthermore, I found that finite values of the second-neighbor (J_2) and ring (K) exchange are necessary to destabilize the DSL, highlighting its resilience to further interactions [3].

To characterize the DSL of this SU(6) symmetric model, I calculated the $S(\mathbf{k},\omega)$ with the VMC method, and compared these results with the non-interacting mean-field calculations. In the SU(6) case, the distribution of the spectral weights in the $S(\mathbf{k},\omega)$ shows a much better agreement between the variational and the mean-field calculations than in the SU(4) or SU(2) cases. I attribute the decreasing difference between the two approaches to the weakening of the fluctuations beyond the mean-field approximation as the SU(N) symmetry increases. To characterize the thermodynamic limit, I calculated the $S(\mathbf{k},\omega)$ in the mean-field approach for an extensive system and found that the spectrum is a gapless continuum of fractionalized excitations [3].

These findings may help experimental identification of Dirac spin liquids, particularly in ultracold atom systems on optical lattices and spin-orbit-coupled materials.

1. D. Vörös and K. Penc, *Dynamical structure factor of the SU(3) Heisenberg chain: Variational Monte Carlo approach*, Physical Review B **104** 184426/1-19 (2021).

2. D. Vörös and K. Penc, *Dynamical structure factor of the SU(4) algebraic spin liquid on the honeycomb lattice*, Physical Review B **108** 214407/1-10 (2023) .

3. D. Vörös, P. Kránitz and K. Penc, *The algebraic spin liquid in the SU(6) Heisenberg model on the kagome lattice*, Physical Review B **110** 144437/1-29 (2024)