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THESIS BOOKLET

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

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Background

The traditional description of phase transitions, developed by Landau, relies on the concept of symmetry breaking. Each distinct phase is associated with a particular symmetry group, and a phase transition is accompanied by a symmetry breaking, in which the symmetry group of one phase is the subset of the symmetry group of the other phase. In this way, concepts like order parameters—quantities that vanish above the critical temperature but acquire a finite value below it—emerged as the universal hallmark of both classical and quantum phase transitions. In Landau's theory, all classical and quantum phase transitions arise from a form of symmetry breaking.

This well-established paradigm was challenged with the discovery of the fractional Quantum Hall effect [1], where multiple distinct phases share the same conventional symmetries. Realizing that such states of matter could not be understood within the symmetry-breaking framework, physicists began searching for "hidden" quantum orders that could distinguish these phases.

Quantum spin liquids (QSLs) represent a typical setting for these novel ideas in Mott insulators. A QSL is the ground state of a quantum spin system that remains fully symmetric—concerning the symmetries of the underlying lattice and of the Hamiltonian. Consequently, QSLs exhibit no conventional magnetic order of any kind (e.g. ferromagnetic or antiferromagnetic). While magnetically ordered ground states usually have bosonic excitations, like the spin-1 magnon, QSLs have fractionalized fermionic excitations, as the spin-$1/2$ spinons. The splitting of the bosonic excitation to a pair of fermionic quasiparticles is called fractionalization. Therefore, the existence of the QSL ground state and the fractionalized excitations is directly measurable through the dynamical spin structure factor, if at the lowest excitation energies we observe a continuum (implicating a pair of quasiparticles) instead of a single branch.

A promising approach to characterizing hidden quantum orders at the mean-field level involves the concept of the projective symmetry group (PSG). When the fluctuations beyond mean-field theory are weak, the mean-field quantum order (protected by the PSG) becomes the quantum order of the real ground state [2, Sec. 9.9.1]. If the mean-field one-particle energy spectrum is gapped, the quantum order is called topological order, and is characterized by the ground state degeneracy [3]. If the one-particle energy spectrum is gapless, then the quantum order is characterized by the existence and location (in reciprocal space) of gapless excitation towers in the dynamical spin structure factor [2, Sec. 9.10.2]. Analogous to symmetry breaking protecting gapless excitations following Goldstone's theorem [4, Sec. 6.1], certain PSGs can protect gapless fermionic excitations and their reciprocal-space locations [2, Sec. 9.10.2]. Experimentally, the dynamical spin structure factor provides a tool to identify a gapless quantum spin liquid ground state [2, Sec. 9]. Quantum phase transitions can occur without conventional symmetry breaking, driven instead by changes in the PSG itself.

One-dimensional spin systems are archetypal examples of quantum spin liquids, where strong quantum fluctuations suppress all forms of magnetic order. In contrast, stabilizing a quantum spin liquid in two-dimensional systems is far more challenging and often requires enhanced fluctuations. Such enhancements can be achieved by geometric frustration (e.g., on the triangular or kagome lattice) or by introducing further-neighbor interactions. Another route is to enlarge the spin symmetry group, considering SU(N) or Sp(N) models with $N > 2$ [5], which increases quantum fluctuations and thereby helps to stabilize quantum spin liquids.

Aims

In this thesis, we seek new avenues to stabilize and characterize two-dimensional quantum spin liquids by considering models with enhanced SU($N > 2$) symmetries.

Our primary goal was to calculate the dynamical spin structure factor of the SU(4) Heisenberg model on the honeycomb lattice, which may be realized in α-$ZrCl_3$ [6], where the strong spin-orbital interaction leads to effective $N = 4$ degrees of freedom. The dynamical spin structure factor can help to verify experimentally if the ground state is a Dirac spin liquid [7]. To achieve this, we extended to SU(N) models the dynamical variational Monte Carlo method, previously successfully applied to the SU(2) case [8, 9]. We tested the method by calculating the dynamical spin structure factor of the exactly solvable SU(3) Heisenberg chain in the fundamental representation. Our calculations showed excellent agreement with the Bethe Ansatz, exact diagonalization, and DMRG results.

Next, we explored whether the ground state of the SU(6) Heisenberg model on the kagome lattice could also be a Dirac spin liquid, inspired by earlier studies on the SU(2) case [10]. This model can be realized in optical lattices of ultracold ^{173}Yb isotopes. In the SU(2) case, the dynamical spin structure factor can be measured in optical lattices by Bragg scattering experiments [11]. In the hope that such measurements can be generalized to the SU(6) case, we calculated the dynamical spin structure factor using the dynamical variational Monte Carlo method.

Methods

I implemented a numerical variational Monte Carlo method—originally introduced in Refs. [8, 9] for computing the dynamical spin structure factor of the SU(2) Heisenberg model—and extended it to the SU(N) case. In this method, the ground state is approximated by the Gutzwiller projected Fermi sea, where the Fermi sea is the mean-field ground state, which is optimized to minimize the variational energy of the Heisenberg Hamiltonian.

To approximate the lowest-energy excited states, we first project the Heisenberg Hamiltonian to the subspace of Gutzwiller projected particle-hole excitations of the Fermi sea. Solving the generalized eigenvalue problem in this subspace provides the energies and eigenstates, which allows us to calculate the spectral weights in the dynamical spin structure factor.

The Gutzwiller projector enforces single occupancy on every lattice site, which is necessary to restore the Hilbert space of the Heisenberg model, which was enlarged in the mean-field approximation. For comparison, we also computed the dynamical spin structure factor in the mean-field approximation without applying the Gutzwiller projector—neither on the Fermi sea nor on its particle-hole excitations. As shown in Ref. [12] for the SU(2) Heisenberg model on the triangular lattice, the Gutzwiller projection can create gapless excitations that are absent in the mean-field calculations. The gapless excitations of the mean-field spectrum also appear after Gutzwiller projection, though the spectral weights are shifted to lower energies.

The results of this variational method are expected to provide a good approximation of the dynamical spin structure factor of the Heisenberg model if the fluctuations beyond the mean-field approximation are weak. The fluctuations are often not weak enough in SU(2) symmetric Heisenberg models. However, in Sp($2N$) symmetric Heisenberg models, the fluctuations were shown to vanish in the large N-limit [5]. Our calculations suggest that the enhanced SU(N) symmetry of the Heisenberg Hamiltonian in the fundamental representation has a similar effect on the fluctuations.

Thesis statements

1. I computed the dynamical spin structure factor $S(k,\omega)$ of the SU(3) Heisenberg chain variationally using Gutzwiller projected particle-hole excitations of the Fermi sea. 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 $S(k,\omega)$ to exact diagonalization results for 18 sites, the two-soliton continuum of the Bethe Ansatz, and the DMRG results for 72 sites. Detailed analysis of the finite-size effects shows that the method captures the critical Wess-Zumino-Witten $\mathrm{SU}(3)_1$ behavior and reproduces the correct exponent, except for the size dependence of the spectral weight in the bottom of the conformal tower. The extracted velocity of excitations and the central charge are very close to the exact results. These results are published in Ref. [I.].

2. I computed the dynamical spin structure factor $S(k,\omega)$ of the SU(4) Heisenberg model on the honeycomb lattice variationally, approximating the ground state by the Gutziller projected π-flux Fermi sea (motivated by Ref. [7]), called a Dirac spin liquid. 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 from higher to lower energies, thus emphasizing the lower edge of the continuum. The ratio of the sums $\left(\sum_{\mathbf{k}\in\mathrm{eBZ}} S^{33}_{\mathrm{MF}}(\mathbf{k})\right) / \left(\sum_{\mathbf{k}\in\mathrm{eBZ}} S^{33}(\mathbf{k})\right) = 1 - 1/N$ shows that the correlations are reduced in the mean-field case, since the charge fluctuations reduce the value of the quadratic Casimir operator, appearing in the sum rules. These results are published in Ref. [II.].

3. I proposed the Gutzwiller projected π-flux Fermi sea (another

Dirac spin liquid) as the ground state of the SU(6) Heisenberg model on the Kagome lattice. To reach this conclusion, I investigated the energetical stability of the Dirac spin liquid (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. These results are published in Ref. [III.].

4. To characterize the DSL on the SU(6) kagome lattice, I calculated the dynamical spin structure factor $S(\mathbf{k}, \omega)$ variationally using Gutzwiller projected particle-hole excitations of the π-flux Fermi sea, 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. Based on this similarity, I have studied the $S(\mathbf{k}, \omega)$ in the mean-field approach for an extensive system with 3888 sites and found that the spectrum is a gapless continuum, where the gapless towers are centered at the Γ, Γ', M and M$'$ points in the extended Brillouin zone. The static spin structure factor $S(\mathbf{k})$ shows increased spectral weights in the form of triangular-shaped plateaus around the K$'$ points in the extended Brillouin zone. The static mean-field and the variational results differ in the sum rules and in the form of barely noticeable humps appearing in the variational calculations around the M$'$ points. The real space spin-spin correlations seem to decay algebraically with the distance, with a power between 3 and 4, similarly as in the SU(4) case (see Ref. [7]). These results are published in Ref. [III.].

Publications related to the thesis

I. 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)

II. 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)

III. 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)

Publication not related to the thesis

IV. M. Kormos, D. Vörös, and G. Zaránd, *Finite-temperature dynamics in gapped one-dimensional models in the sine-Gordon family* Physical Review B **106** 205151/1-16 (2022).

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