

A diagrammatic theory of the antiferromagnetic frustrated 2d Heisenberg model

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Abstract. We consider the ground state properties of the two-dimensional spin-1/2 J_1 - J_2 -Heisenberg model on a square lattice. Within a diagrammatic formulation in terms of auxiliary fermions we consider two different approximation schemes. First we use a phenomenological assumption on the width of the pseudofermion spectral function to calculate the magnetization and the correlation length within RPA with qualitatively correct results. Secondly we employ a Functional Renormalization Group formulation to obtain quantitative results on the ground state correlations. We discuss two different projection schemes to account for the auxiliary particle constraint.

Frustrated two dimensional quantum systems attract much interest in condensed matter physics. A generic model to study the effects of frustration is the spin-1/2 J_1 - J_2 -Heisenberg model on a square lattice in two dimensions

$$H = J_1 \sum_{nn} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{nmn} \mathbf{S}_i \cdot \mathbf{S}_j \quad . \quad (1)$$

Here $J_1 > 0$ denotes the interaction between nearest-neighbors and $J_2 \geq 0$ a frustrating next nearest-neighbor exchange. Two limits of the ground state are well understood: For $J_2 = 0$ the model features a Néel-like state with a magnetization of $\sim 60\%$ of the saturation value. In the limit $g = \frac{J_2}{J_1} \rightarrow \infty$ the model decouples into two square lattices where each exhibits Néel order. This results in the so-called Collinear order in which the spins are aligned in stripes along one of the two axes. For intermediate values of g both states become frustrated, causing a decrease of the respective order parameter. Indeed, there is a parameter region $g \approx 0.4 \dots 0.6$ where a phase without magnetic long-range order is expected. The nature of this phase as well as the order of the quantum phase-transitions are still highly controversial issues. Under debate are spin-liquids and valence-bond-solids with dimer or plaquette order. The knowledge about the model mainly stems from exact diagonalization [1], coupled cluster method [2], series expansion [3], Monte Carlo [4] as well as field-theory methods [5].

In this paper we present a different approach to the model. The commutation relations of the spin-operators are neither bosonic nor fermionic, making it impossible to use Wick's theorem and to set up a diagrammatic theory. To resolve this problem we express the spin operators in terms of auxiliary fermions

$$S_i^\mu = \frac{1}{2} \sum_{\alpha\beta} f_{i\alpha}^\dagger \sigma_{\alpha\beta}^\mu f_{i\beta} \quad . \quad (2)$$

Here we introduced two Fermi operators $f_{i\alpha}$, $\alpha = \uparrow, \downarrow$, for every lattice site i ; σ^μ with $\mu = x, y, z$ denotes the Pauli matrices. By construction, this representation has the correct commutation relations. Nevertheless the operator (2) allows states with $S = 0$ and $S = 1/2$. For $S = 1/2$ the site is occupied with one fermion (\uparrow or \downarrow) while the states with $S = 0$ exhibit either no or two fermions. Clearly, states with $S = 0$ are unphysical. Thus for every site i we require the fulfillment of the constraint

$$Q_i = \sum_{\alpha} f_{i\alpha}^\dagger f_{i\alpha} = 1 \quad . \quad (3)$$

We apply two methods to enforce this identity. On the one hand we treat the constraint approximatively by replacing it by the simpler condition $\langle Q_i \rangle = 0$, i.e., we only require the fulfillment *on average*. This can be easily performed by introducing a chemical potential μ , which turns out to be $\mu = 0$ due to particle-hole symmetry of the Hamiltonian. On the other hand, using an approach by Popov and Fedotov [6] the unphysical states can be projected out *exactly*. They introduced a homogeneous, *imaginary* chemical potential $\mu^{ppv} = -\frac{i\pi T}{2}$, where T is the temperature. Using the Hamiltonian $H^{ppv} = H - \mu^{ppv} \sum_i Q_i$ and the full Hilbert-space (including $Q_i = 0, 2$) to derive expectation values of physical observables $\langle A \rangle$, one can show [7] that the contributions of the unphysical states exactly cancel. Although μ^{ppv} vanishes in the limit $T \rightarrow 0$, in principle the exact projection with $\mu = \mu^{ppv}$ and the average projection with $\mu = 0$ may differ even in the limit $T \rightarrow 0$. Nevertheless it can be expected that in the model considered here both projection schemes are identical at $T = 0$ and the simpler average projection becomes exact [7]. In most calculations we restrict ourself to this method.

Inserting the auxiliary fermion representation (2) into (1) yields a Hamiltonian which can be treated with standard Feynman-diagram techniques. Since only terms quartic in the fields appear, the bare fermion-Green's function in real space reads

$$G_{ij\alpha\beta}^0(i\omega) = \frac{1}{i\omega + \mu} \delta_{ij} \delta_{\alpha\beta} \quad ; \quad \mu = -\frac{i\pi T}{2} \text{ or } \mu = 0 \quad . \quad (4)$$

$\omega = (2n + 1)\pi T$ are the fermionic Matsubara frequencies, i, j are site indices and α, β spin indices. It should be emphasized that the Green's function is always a strictly local entity, i.e. $\propto \delta_{ij}$.

The simplest approximation scheme for an analytical approach is the self-consistent Hartree approximation, i.e., the magnetic mean-field theory, see figure 1. (Note that the Fock approximation induces forbidden fermion hopping and will therefore be excluded here.)

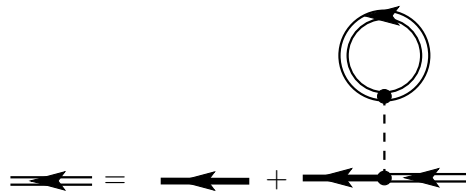


Figure 1. Diagrammatic representation of the Hartree approximation. The full line is the bare Green's function G^0 , Eq.(4), the double-stroke line the self consistent one. The dashed line represents the interaction J_1 or J_2 and the dots are Pauli matrices $\times 1/2$.

Solving the self-consistent equation for magnetizations $M_{N\acute{e}el} = N^{-1} \sum_i \langle S_i^z \rangle (-1)^{i_x + i_y}$ and $M_{Col} = N^{-1} \sum_i \langle S_i^z \rangle (-1)^{i_x}$, corresponding to N\'eel and Collinear order, reproduces at $T = 0$ the results of the classical large-spin limit: For $0 \leq g < 1/2$ the system is maximal N\'eel-ordered. At $g = 1/2$ the system undergoes a first order transition to a maximal Collinear ordered phase which exists for all $g > 1/2$. This holds for both projection schemes.

We now present a simple phenomenological theory for the ground state which treats the system beyond the Hartree approximation and which gives qualitatively good results. The fermions' spectrum of the bare (free) propagator used in the Hartree scheme is a δ -function,

$\rho(\omega) = \delta(\omega)$. In a more realistic description, fermions scatter and the corresponding quasi particles obtain a finite lifetime. This results in a broadening of the spectrum, described by some width γ . We assume that the spectrum is Lorentz-shaped $\rho(\omega) = -\frac{1}{\pi} \text{Im}G(\omega + i\delta) = \frac{\gamma}{\pi} \frac{1}{\omega^2 + \gamma^2}$, with the phenomenological damping parameter γ . Since in the limit $g \rightarrow \infty$ the system consists of two independently Néel-ordered sublattices, the relation $\frac{\gamma}{J_1}|_{J_2=0} = \frac{\gamma}{J_2}|_{J_1=0}$ holds. This can be satisfied by the form $\gamma(J_1, J_2) = \tilde{\gamma} J_1 \sqrt{1 + g^2}$ used in the following. Inserting this new propagator instead of the free propagator into figure 1, one obtains magnetizations as shown in figure 2. An increase of the width $\tilde{\gamma}$ reduces the magnetizations, especially in the region of high frustration around $g = 1/2$. In particular, for high enough $\tilde{\gamma}$, a non-magnetic phase emerges. Again, both projection methods produce the same results.

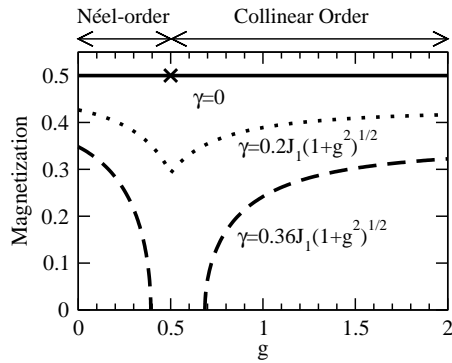


Figure 2. Staggered and Collinear magnetization versus g for various widths $\tilde{\gamma}$. Full line: $\tilde{\gamma} = 0$, dotted line: $\tilde{\gamma} = 0.2$, dashed line $\tilde{\gamma} = 0.36$

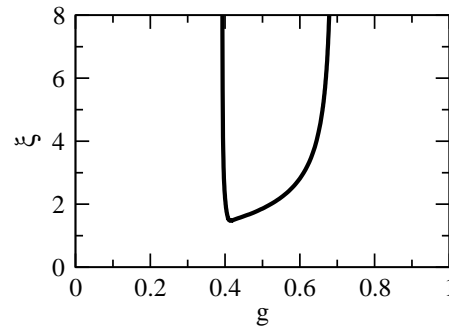


Figure 3. Correlation length in the non-magnetic phase in units of the lattice spacing as a function of g for $\tilde{\gamma} = 0.36$.

In order to calculate the corresponding susceptibility and correlation function, an RPA scheme is applied. Note that the particle-conserving property of this approximation is essential in our auxiliary fermion description. We calculated the correlation function for a width $\tilde{\gamma} = 0.36$ in the non-magnetic phase. For this width the quantum phase-transitions occur at reasonable values g , i.e., $g \approx 0.39$ and $g \approx 0.69$. From the correlation function we extracted the correlation length ξ , see figure 3. It clearly shows divergences at the phase-transitions where the magnetism sets in, but gets rather small in the vicinity of $g = 0.4$, i.e., down to ≈ 1.5 .

The approximation presented so far is a good tool to extract the qualitative behavior of many physical observables, but the width γ of the spectrum is not calculated. Unfortunately summing up diagrammatic contributions of the Greens function to obtain reasonable values for the width is a difficult task. Remember that no small parameter exists in our model. Thus results strongly depend on the diagram classes in use. A controlled way to handle a large class of terms is given by the Functional Renormalization Group (FRG). This method describes the flow of the

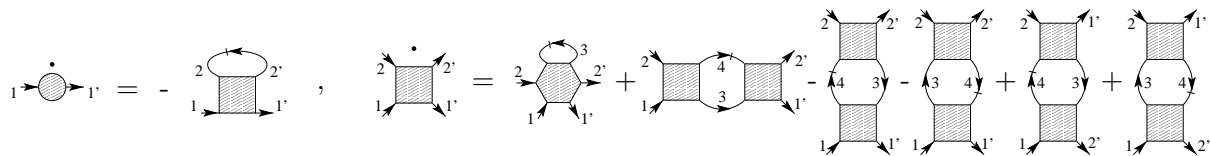


Figure 4. FRG flow equations for the self energy $\Sigma^\Lambda(i\omega)$ and the two-particle vertex. The slashed line is the single scale propagator $S^\Lambda(i\omega)$, the line without slash the Green's function $G^\Lambda(i\omega)$ and the dots denote derivatives $\frac{d}{d\Lambda}$.

vertex functions with respect to an artificial frequency cutoff Λ . The corresponding differential equations for the self-energy and the two-particle vertex are shown in figure 4 in diagrammatic form. A closed set of equations is obtained by neglecting the three-particle vertex (first term on the right side of the second equation in figure 4) and higher vertices. Here the cutoff dependent Green's function is given by $G^\Lambda(i\omega) = \frac{\Theta(|\omega|-\Lambda)}{i\omega - \Sigma^\Lambda(i\omega)}$. In the standard formulation [8] the single scale propagator reads $S^\Lambda(i\omega) = \frac{\delta(|\omega|-\Lambda)}{i\omega - \Sigma^\Lambda(i\omega)}$. In order to improve the fulfillment of Ward-identities, which are important in view of particle conservation, a different approach [9] is applied. We use a modified "single scale" propagator given by $\tilde{S}^\Lambda(i\omega) = \frac{\delta(|\omega|-\Lambda)}{i\omega - \Sigma^\Lambda(i\omega)} - \frac{\Theta(|\omega|-\Lambda)}{(i\omega - \Sigma^\Lambda(i\omega))^2} \frac{d}{d\Lambda} \Sigma^\Lambda(i\omega)$ and solve the flow equations with all frequency dependencies for a discrete set of frequencies. In order to get a finite number of equations we omit all two-particle vertices in which the two in-going (or out-going) legs exceed a maximal spacial distance. Connecting the legs of the two-particle vertex we calculate the correlation function from which in turn the correlation length can be derived. Results for the flowing correlation length are shown in figure 5.

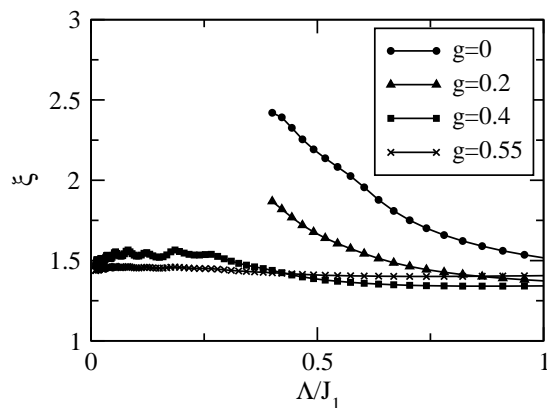


Figure 5. Flowing correlation length $\xi(\Lambda)$ for different values of the frustration $g = \frac{J_2}{J_1}$.

For a strong frustration $g = 0.55$ we observe a smooth flow towards $\Lambda = 0$. Since the correlation length stays finite for $\Lambda \rightarrow 0$ we identify a non-magnetic phase in this parameter region. In correspondence with the phenomenological theory described above we obtain a small correlation length $\xi = 1.46$. However, for a smaller $g = 0.4$ the flow is unstable and shows oscillations, which result from the discretization of the frequencies. We interpret this behavior as the proximity to magnetic order. A smooth divergence in the region where magnetism is expected seems hard to resolve due to a numerically unstable flow. For $g = 0$ an increasing correlation length is visible until the numerics break down at $\Lambda \approx 0.4J_1$. A similar behavior is observed for an approach to the Collinear phase. FRG calculations in the J_1 - J_2 -model are discussed in much more detail in an upcoming publication.

To conclude, we developed a simple phenomenological theory to describe the qualitative behavior of the J_1 - J_2 -model. Quantitative results are obtained within FRG. Here a non-magnetic phase is clearly seen in the parameter range $\frac{J_2}{J_1} \approx 0.4 \dots 0.7$.

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