

Low temperature long-range ordering of a classical XY spin system with bilinear-biquadratic exchange Hamiltonian

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Abstract

We investigate low temperature long-range ordering of a classical XY spin system with bilinear and biquadratic exchange interactions, J_1 and J_2 , respectively, on stacked triangular lattice by histogram Monte Carlo simulations. Focus is laid on determination of phase boundaries, nature of transitions, and magnetic structures in the respective phases. Negative J_1 and/or J_2 induce lattice geometry frustration that can be either relaxed or enhanced, depending on the signs and strengths of both exchanges. Moreover, the exchanges can also mutually compete. Hence, the resulting low temperature phase diagram in $J_1 - J_2$ parameter space features several peculiar phases, including highly disordered ones in the regions of the coexistence of a non-frustrated exchange with a frustration inducing one.

Key words: planar Heisenberg model; bilinear-biquadratic exchange; frustration; phase transition

1. Model and methods of calculation

We consider the following Hamiltonian on stacked triangular lattice

$$H = -J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - J_2 \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j)^2, \quad (1)$$

where $\mathbf{S}_i = (S_i^x, S_i^y)$ is a two-dimensional unit vector at the i th lattice site and the sum $\langle i,j \rangle$ runs over all its nearest neighbors. J_1 and J_2 are bilinear and biquadratic exchange interactions, respectively, and we will consider four cases: (i) $J_1 > 0, J_2 > 0$, (ii) $J_1 < 0, J_2 < 0$, (iii) $J_1 < 0, J_2 > 0$, and (iv) $J_1 > 0, J_2 < 0$.

At finite temperatures we run standard and histogram Monte Carlo (MC) simulations using lattices of linear dimensions $L = 12, 18, 24$ and 30 , periodic boundary condition, and up to 4×10^6 MC steps per spin (MCS/s) for calculating averages and 2×10^6 MCS/s for thermalization. We calculate physical quantities that give us relevant information on critical behavior such as the appropriate long-range order (LRO)

parameters, the internal energy, the specific heat, the susceptibility, the fourth-order energy and LRO parameters cumulants, etc. (see [1] for definitions). With some precautions the simulations are feasible down to very low temperatures ($t = k_B T / |J_2| \approx 0.001$). Ground states (GS) are determined by extrapolation of phase boundaries to $t = 0$, observation of snapshots near GS, and crosschecked by analytical means such as seeking energetically stable configurations.

2. Ground state phase diagram

(i) $J_1 > 0, J_2 > 0$. This is the simplest case with no frustration present. As long as J_1 is finite, GS is always ferromagnetic (FM).

(ii) $J_1 < 0, J_2 < 0$. This case is more complicated because of the presence of both the in-plane geometrical frustration, due to the lattice geometry and antiferromagnetic (AFM)/antiferroquadrupolar (AFQ) exchanges, and the out-of-plane competition between the two exchanges. For $J_1/J_2 > 2$, GS shows the chiral AFM LRO characterized by the 120° and 180°

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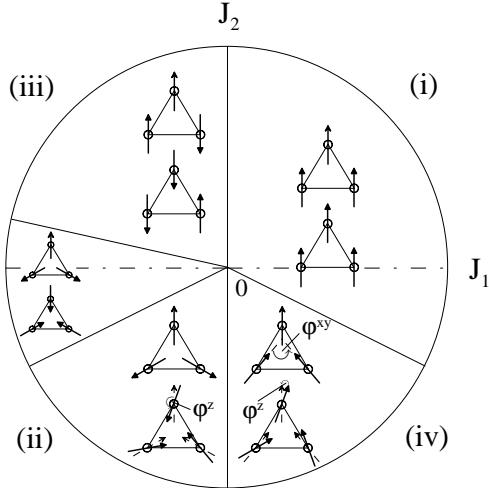


Fig. 1. Ground state phase diagram in $J_1 - J_2$ space with schematical spin alignments in two adjacent (up-down) planes.

spin arrangements within and between planes, respectively, i.e., just like in the case with $J_2 = 0$. However, if $0 < J_1/J_2 < 2$ the system displays an incommensurate (IC) arrangement in the stacking direction due to the exchange competition. This arrangement is characterized by a non-universal turn angle φ^z between spins of two successive AFM layers, the absolute value of which varies continuously with J_1/J_2 but its sign is arbitrary due to the two-fold degeneracy ($\pm\varphi^z$).

(iii) $J_1 < 0, J_2 > 0$. Here, we are concerned with the system which, besides the in-plane geometrical frustration due to $J_1 < 0$, displays an additional frustration due to the in-plane competition between the non-collinear chiral and collinear ferroquadrupolar (FQ) alignments favored by the bilinear and bi-quadratic forces, respectively. Like in the case (ii), if $|J_1|/J_2$ is large enough (> 4.5), the system shows the chiral AFM LRO. For $0 < |J_1|/J_2 < 4.5$, however, the GS arrangement is AFM (antiparallel) only in the stacking direction. Within planes there is only FQ order present. The transition at $|J_1|/J_2 = 4.5$ is pronouncedly first order, accompanied by abrupt changes in physical quantities.

(iv) $J_1 > 0, J_2 < 0$. This last case is the most complicated since the two exchanges compete in both in-plane and out-of-plane directions and induce a high degree of frustration. For $|J_1|/|J_2| > 2$, the system shows standard FM LRO, but within $0 < |J_1|/|J_2| < 2$ due to considerable frustration the system is highly disordered. The out-of-plane spin arrangement is IC, similar to the one in case (ii). Here, however, also the in-plane arrangement is non-collinear. Observing snapshots near GS, we could see triangular plaquettes of canted in-plaquette FM order with "2 spins in 1 spin

out" and "1 spin in 2 spins out" patterns, however, with no order among such plaquettes. Minimizing the out-of-plane and in-plane internal energy contributions, we can determine the respective GS turn angles φ^z and φ^{xy} as solutions of the equations: $2\cos(\varphi^z) + \alpha = 0$ and $\sin(2\varphi^{xy}) + (1 + \alpha)\sin(\varphi^{xy}) + \alpha\sin(\varphi^{xy}/2) = 0$, where $\alpha = J_1/J_2$. From the former equation we can also determine φ^z in the case (ii). The respective GS phases are shown in Fig. 1.

3. Finite temperature effects

In above we could see that each of the frustrated systems showed at sufficiently low $|J_1/J_2|$ some degree of GS disorder due to frustration induced degeneracy. Especially in the highly frustrated systems (iii) and (iv), it is interesting to observe what happens at finite temperatures. In the case (iii), for $0 < |J_1/J_2| \leq 3.1$ the GS degeneracy is partially lifted thanks to thermal excitations that facilitate the in-plane AFM ordering by providing AFM forces with some freedom to satisfy their needs. As a result, spins align on plaquettes in a quasi-collinear two-fold degenerated pattern: one spin "up" and two deviated spins "down" (Fig. 2). For $3.1 < |J_1|/J_2 < 4.5$, there is a strong first-order transition to the 120° chiral AFM LRO phase.

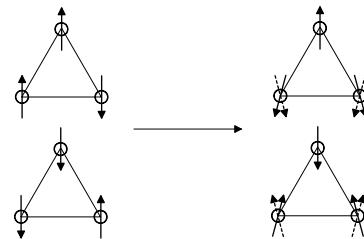


Fig. 2. GS (left) and excited (right) spin alignments in case (iii).

In the most frustrated case (iv), for $0 < |J_1|/|J_2| < 2$, the degeneracy is being lifted by increasing temperature in several steps. First, the canted FM plaquettes start showing FM order within planes, then the out-of-plane degeneracy is lifted, producing canted FM LRO in all directions, before the conventional collinear FM LRO sets in. All this occurs at very low temperatures. For example, at $|J_1/J_2| = 1$, the respective transition temperatures are: $T_1 \approx 0.0045 T_P$, $T_2 \approx 0.0075 T_P$, $T_3 \approx 0.083 T_P$, where T_P is transition temperature to paramagnetic phase (to be compared to the relatively high $T_1 \approx 0.513 T_P$ in case (iii)).

References

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