XY checkerboard antiferromagnet in external field

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Abstract. Ordering by thermal fluctuations is studied for the classical XY antiferromagnet on a checkerboard lattice in zero and finite magnetic fields by means of analytical and Monte Carlo methods. The model exhibits a variety of novel broken symmetries including states with nematic ordering in zero field and with triatic order parameter at high fields.

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1. Introduction

A huge degeneracy of classical ground states in geometrically frustrated magnets can be lifted by quantum or thermal fluctuations via a so called order by disorder effect [1]. In the present work we study the thermal order by disorder effect for the XY antiferromagnet on a checkerboard lattice. This lattice is a two-dimensional network of corner-sharing squares with crossings, which are topologically equivalent to tetrahedra, see Fig. 1. The present model can, therefore, be relevant to real pyrochlores with the easy-plane type anisotropy Er₂Ti₂O₇ and Er₂Sn₂O₇ [2] and also have an experimental realization as an array of the Josephson junctions or a superconducting wires network in transverse magnetic field [3].

The considered model is described by the Hamiltonian
\[
\hat{H} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_i \mathbf{H} \cdot \mathbf{S}_i ,
\]
where \(\mathbf{S}_i = (\cos \varphi_i, \sin \varphi_i)\) are the classical planar spins and \(\mathbf{H} = (H, 0)\) is in-plane magnetic field. The sum is over nearest-neighbors pairs on a checkerboard lattice and \(J > 0\) is an antiferromagnetic coupling constant. The Hamiltonian can be expressed as a sum over elementary plaquettes (squares with crossings):
\[
\hat{H} = \frac{1}{2} \sum_p (J \mathbf{S}_p^2 - \mathbf{H} \cdot \mathbf{S}_p) - JN ,
\]
where \(\mathbf{S}_p = \sum_{i \in p} \mathbf{S}_i\) is the total magnetisation of a plaquette, \(N\) is the number of sites on the lattice and \(N_p = \frac{1}{2}N\) is the number of plaquettes. Minimizing energy of a single plaquette one obtains the classical constraint
\[
\mathbf{S}_p = \mathbf{H}/(2J) .
\]
The minimal total energy is reached if the above constraint is satisfied on every plaquette. In the field range $0 \leq H \leq H_{\text{sat}} = 8J$ the ground state of the model remains underconstrained and infinitely degenerate with a finite entropy. This huge degeneracy is determined by two factors: (i) possible basis spin quartets, which obey the classical constraint, are parametrized by two continuous variables and (ii) by various periodic and aperiodic spin structures formed with the same basis quartet. The latter property can be seen by looking at the Fourier transform of the interactions on the checkerboard lattice [4], which has a flat momentum-independent branch with minimal energy.

2. Thermal order by disorder effect

Since the degeneracy of the classical ground state is a consequence of lattice topology rather than being a symmetry imposed property, various classical ground state configurations have different excitation spectra. At finite temperatures magnetic system spans a phase volume in the vicinity of the ground state manifold. Due to a varying density of excitations, the system can be effectively trapped in the neighbourhood of certain ground states. Such an ergodicity breaking leads to a lifting of zero-$T$ degeneracy of a frustrated magnet and to thermal order by disorder selection. The statistical weights of different ground state configurations $\psi$ are given by $w[\psi] \sim \exp(-F[\psi]/T)$, where $F[\psi]$ is the partial free energy obtained by integrating out 'fast' excitation modes. The minimum of $F[\psi]$ ensures that a macroscopic system is trapped in the vicinity $\psi_{\text{min}}$ and probability to find it in another classical ground state is vanishingly small.

To find which spin configurations are favoured by thermal fluctuations we start with a simple perturbative treatment over the mean-field result. In the ground state configuration a magnitude of a local field derived from Eq. (2) is the same $H_{\text{loc}} = 2J$ for all sites and all external fields $0 \leq H \leq H_{\text{sat}}$. The harmonic spin-wave Hamiltonian is expressed as

$$\hat{H}_2 = -H_{\text{loc}} \sum_i S_i^z + J \sum_{\langle ij \rangle} S_i^y S_j^y \cos \theta_{ij}, \quad S_i^z \approx 1 - \frac{1}{2} S_i^{y^2},$$

(4)

where components of every spin are taken in its local coordinate frame and $\theta_{ij}$ is an angle between neighbouring spins. The first term in $\hat{H}_2$, which describes uncorrelated fluctuations of individual spins with $\langle S_i^{y^2} \rangle = T/H_{\text{loc}}$, is taken as an unperturbed spin-fluctuation Hamiltonian, whereas the second term is a perturbation $\hat{V}$. The correction to the free-energy is given by $\Delta F = -(\hat{V}^2)/2T$:

$$\Delta F = -(T/8) \sum_{\langle ij \rangle} \cos^2 \theta_{ij} = -(T/8) \sum_{\langle ij \rangle} (S_i \cdot S_j)^2.$$  

(5)

Thermal fluctuations produce, therefore, an effective biquadratic exchange, which lifts the zero-$T$ degeneracy in favour of maximally collinear states with the largest number of $\cos \theta_{ij} = \pm 1$. The harmonic Hamiltonian can be, of course, diagonalized with the help of the Fourier transform to obtain the spin wave modes $\omega_n^k$ and their contribution to the free-energy:

$$\Delta F_2 = T \sum_n \sum_k \ln(\omega_n^k / \pi T).$$

(6)

The problem is reduced to minimization of the sum in (6). Still the real-space second order perturbation result appears to give a correct first insight especially for
multisublattice configurations with \( n > 2 \), when exact diagonalization of \( \hat{H}_2 \) becomes increasingly cumbersome.

An additional complication of highly frustrated magnets stems from a presence of several branches of zero modes: \( \omega_k^m \equiv 0 \), in which case Eq. (5) is not anymore correct. Instead the low-\( T \) contribution to the free energy becomes:

\[
\Delta F = \left( N_2/2 + N_4/4 \right) T \ln(J/T) + T \sum_{n \neq m, k} \ln \omega_k^m / J + T f_4 ,
\]

where \( N_2 \) is the number of usual harmonic or quadratic modes, \( N_4 \) is the number of zero or soft modes, and \( f_4 \) is a contribution from interaction between soft modes and their interaction with quadratic modes. In order to estimate the last term one has to solve a nonlinear problem, which is, generally, a very complicated task. However, a partial selection between various spin configuration can be done on a basis of the leading \( T \ln(J/T) \) term. If the total number \( N_2 + N_4 \) is fixed (\( = N \) for the XY checkerboard antiferromagnet), then, the free energy is minimal for states with the maximum number of soft modes. The number of soft modes can be found either from direct diagonalization of \( \hat{H}_2 \) or from geometric consideration, which assigns a local soft mode to every void (empty square) with all spins around it being parallel or antiparallel to each other [5, 6, 7]. Thus, the soft modes act similar to harmonic excitations and stabilize collinear states.

3. Zero field behaviour

At zero magnetic field the ground state constraint (3) specifies configurations with \( S_p = 0 \) on every plaquette. Such configurations can be constructed either from noncollinear or collinear spin quartets. As was argued above, thermal fluctuations tend to select maximally collinear states with two up- and two down-spins on an arbitrarily chosen axis in the XY plane. The gauge transformation \( S_i^{\text{down}} = -S_i^{\text{down}} \) maps \( \hat{H}_2 \) for an arbitrary collinear state on the same reference harmonic Hamiltonian. Every collinear state has, therefore, the same harmonic spectrum and the same number of zero (soft) modes \( N_4 = \frac{1}{2} N \). Hence, the specific heat of a collinear state is \( C = \frac{3}{8} \). All terms in the low-\( T \) expression for the free energy (7) except the last one coincide for all collinear states. Our estimate indicates that the Néel state with the ordering wavevector \( \mathbf{Q} = (\pi, \pi) \) on the original square lattice has the lowest anharmonic contribution \( f_4 \) among all translationally symmetric states. This, however, does not necessarily mean an appearance of a quasi long-range order at \( \mathbf{q} = \mathbf{Q} \) when \( T \to 0 \). So called weathervane defects [5] or wondering (rough) domain walls [8] have been considered as a source of disorder for the kagome antiferromagnet. For the XY checkerboard antiferromagnet there are no zero-width domain walls and only weathervane defects can destroy a quasi long-range translational order. They cost zero classical energy and increase the free-energy by \( \Delta F_d \sim \varepsilon_d T \). A finite \( T \)-independent density of such defects can be estimated as \( n_d \simeq (1 + e^{\varepsilon_d})^{-1} \) by neglecting interaction between defects. These defects can destroy the true long-range order if their concentration exceeds the percolation threshold on the corresponding lattice. In this case only nematic correlations described by a traceless second-rank tensor \( O_{\text{nem}}^{\alpha\beta} = \langle S_1^\alpha S_1^\beta \rangle - \frac{1}{2} \delta^{\alpha\beta} \) will be present at low temperatures.
In the absence of analytical theory to deal with this sort of behaviour we have tried to derive the necessary information from Monte Carlo simulations. We have calculated squares of the two relevant low-\(T\) order parameters:

\[
S(Q) = \frac{1}{N^2} \sum_{i,j} \langle S_\alpha^i S_\beta^j \rangle e^{iQ(r_i - r_j)}, \quad O_{\text{nem}}^2 = \frac{1}{N^2} \sum_{i,j} \langle S_\alpha^i S_\beta^j S_\alpha^j S_\beta^j \rangle - \frac{1}{2}.
\]  

(8)

The results are presented in Fig. 1. There is a clear signature of the nematic order seen by the enhancement of \(O_{\text{nem}}^2(N)\) at low temperatures. The Néel order parameter reaches only very small values and does not show any appreciable enhancement. Considering a change in the scaling behaviour of the nematic order parameter \(O_{\text{nem}}^2(N) \sim 1/N^\alpha\) from \(\alpha = 1\), short-range correlations, at high temperatures to \(\alpha < 1\), power-law correlations, at low temperatures we estimate the Kosterlits-Touless transition temperature as \(T_{\text{KT}} = 0.014(2)J\).

4. Finite field phases

In external magnetic fields \(0 < H < H_{\text{sat}}\) the ground states with intermediate magnetisation [3] are, generally, noncollinear, except for \(H = \frac{1}{2}H_{\text{sat}}\), when a collinear ‘\(uuud\)’ state, Fig. 2b, belongs to the ground state manifold. Selection of the \(uuud\) states by thermal fluctuations leads to a 1/2-magnetization plateau, which is similar to a 1/3-plateau of a classical kagome antiferromagnet [7]. At all other fields only a partial collinearity is possible in the classical ground state. Geometric consideration suggests two prime candidate states shown in Fig. 2. The first canted state, Fig. 2a, exists
in the whole range of fields and does not break remaining spin reflection symmetry about the field direction. The second partially collinear state, Fig. 2c, with three identical sublattices appears only for $H > \frac{1}{2}H_{\text{sat}}$ and does break the mirror symmetry. It is easy to check that the fluctuation induced biquadratic exchange (5) favours a ‘more’ collinear state with broken reflection symmetry $\Delta F = -(T/8)\left[3 + \frac{1}{2}(8h^2 - 5)^2\right]$, $h = H/H_{\text{sat}}$ over a ‘less’ collinear canted state $\Delta F = -(T/8)\left[2 + 4(2h^2 - 1)^2\right]$ in the whole range of existence of the former state.

The translational degeneracy of the high-field partially collinear states is similar to the degeneracy of the $uuud$ states and corresponds to the dimer coverings of a square lattice [9], the total number of such states being $\sim 1.157^N$. The problem of lifting translational degeneracy for the $uuud$ states is similar to the zero-field case discussed above. Also, the $uuud$ have the same specific heat $C = \frac{3}{8}$. For the partially collinear states there are additional features in the thermal order by disorder effect. A general partially collinear state does not have soft modes. Soft modes, corresponding to all parallel spins around an empty square, exist, nevertheless, for certain translational patterns. The maximum number of soft modes $N_4 = N/4$ appears for a state shown in Fig. 2d, which corresponds to a columnar arrangement of effective dimers. Such a translational pattern has the lowest $T \ln(J/T)$ contribution to the free energy. However, for all temperatures $T \geq 0.001J$ accessible with our Monte Carlo code we did not find a nonvanishing value of the structure factor corresponding to the
this state. Thus, there is no a conventional Ising order parameter \( \langle S^y_i \rangle \equiv 0 \), \( \forall i \) in the high-field partially collinear state. Instead an Ising reflection symmetry is broken by a unique triatic order parameter:

\[
T_{yyy} = \langle S^y_i S^y_i S^y_i \rangle .
\]

(9)

For Monte Carlo simulations of the XY checkerboard antiferromagnet we have used the standard Metropolis algorithm discarding \( \sim 10^5 \) Monte Carlo steps per spin (MCS) to reach thermal equilibrium and, then, average observables over \( 10^6 \)–\( 10^7 \) MCS. The lattice sizes were up to \( N = 1024 \). In order to estimate statistical errors, all results have been averaged over 10–20 runs. The field dependence of the specific heat \( C \) is shown in Fig. 2 for \( T = 0.002J \). \( C \) starts at value, which is very close to analytically predicted \( \frac{3}{8} \). In applied field the system loses gradually soft modes up to \( H = 0.5H_{sat} \), where \( uuud \) state with \( C = \frac{3}{8} \) appears. The peaks in the specific heat at \( H_{c1} = 4.15J \) and \( H_{c2} = 6.8J \) indicate the phase transitions to a high-field state with broken reflection symmetry. The order parameters for this state are presented in the bottom right panel of Fig. 2. The square of the triatic order parameter \( T_{yyy} \) is nonzero between \( H_{c1} \) and \( H_{c2} \). It shows a good statistical averaging and very little finite size dependence: results for smaller clusters fall on top of the presented data for \( N = 1024 \). The inset shows \( S^y(q) \) with \( q = (\pi, \pi) \) on a new lattice built from one sort of tetrahedra, which should be nonzero if the long-range order corresponding to Fig. 2d is present. The obtained data show that \( S^y(q) \equiv 0 \) in the thermodynamic limit. Thus, the high-field state is described by the triatic order parameter \( T_{yyy} \) which makes the checkerboard lattice to be similar to a classical kagome antiferromagnet [7]. Our results suggest that the triatic state survives up to \( T \sim 0.015J \).

In conclusion, we have investigated the low temperature phases of the XY checkerboard antiferromagnet in strong external fields. We have found that thermal fluctuations stabilize interesting phases with new type of broken symmetries: nematic order at \( H = 0 \) and triatic order [9] in the field range \( \frac{1}{2}H_{sat} < H < H_{sat} \). Further theoretical investigations should focus on a unique \( H-T \) diagram of this model.

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References

[1] J. Villain et al., J. Phys. (Paris) 41, 1263 (1980); E. F. Shender, Sov. Phys. JETP 56, 178 (1982); C. L. Henley, Phys. Rev. Lett. 62, 2056 (1989).
[2] H. W. J. Blöte et al., Physica 43, 549 (1969); M. J. Harris et al., J. Magn. Magn. Mater. 177, 757 (1998); J. D. M. Champion et al., Phys. Rev. B 68, 020401 (2003).
[3] P. Matinoli and C. Leemann, J. Low Temp. Phys. 118, 699 (2000); M. J. Higgins, Y. Xiao, S. Bhattacharyya, P. M. Chaikin, S. Sethuraman, R. Bojko, and D. Spencer, Phys. Rev. B 61, 894 (2000).
[4] B. Canals, Phys. Rev. B 65, 184408 (2002).
[5] J. T. Chalker, P. C. W. Holdsworth, and E. F. Shender, Phys. Rev. Lett. 68, 855 (1992); I. Ritchey, P. Chandra, and P. Coleman, Phys. Rev. B 47, 15342 (1993).
[6] R. Moessner and J. T. Chalker, Phys. Rev. B 58, 12049 (1998).
[7] M. E. Zhitomirsky, Phys. Rev. Lett. 88, 057204 (2002).
[8] S. E. Korshunov, Phys. Rev. B 65, 054416 (2002).
[9] R. Moessner and S. L. Sondhi, Phys. Rev. B 63, 224401 (2001).