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2004 J. Phys.: Condens. Matter 16 S759

(http://iopscience.iop.org/0953-8984/16/11/026)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **16** (2004) S759–S764 PII: S0953-8984(04)74224-1

An XY checkerboard antiferromagnet in an external field

Benjamin Canals[1] **and M E Zhitomirsky**[2]

[1] Laboratoire Louis Néel, CNRS, 25 avenue des Martyrs, Boite Postale 166, 38042 Grenoble Cedex 9, France
[2] Commissariat á l'Energie Atomique, DSM/DRFMC/SPSMS, 17 avenue des Martyrs, 38054 Grenoble Cedex 9, France

Received 7 January 2004
Published 4 March 2004
Online at stacks.iop.org/JPhysCM/16/S759 (DOI: 10.1088/0953-8984/16/11/026)

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.

(Some figures in this article are in colour only in the electronic version)

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 figure 1. The present model can, therefore, be relevant to real pyrochlores with the easy-plane-type anisotropy, $Er_2Ti_2O_7$ and $Er_2Sn_2O_7$ [2], and can also have an experimental realization as an array of Josephson junctions or a superconducting wire network in a transverse magnetic field [3].

The model considered is described by the Hamiltonian

$$\hat{\mathcal{H}} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_i \mathbf{H} \cdot \mathbf{S}_i, \tag{1}$$

where $\mathbf{S}_i = (\cos\varphi_i, \sin\varphi_i)$ are the classical planar spins and $\mathbf{H} = (H, 0)$ is the in-plane magnetic field. The sum is over nearest-neighbour 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):

$$\hat{\mathcal{H}} = \tfrac{1}{2} \sum_p^{N_\mathrm{p}} (J\mathbf{S}_\mathrm{p}^2 - \mathbf{H} \cdot \mathbf{S}_\mathrm{p}) - JN, \tag{2}$$

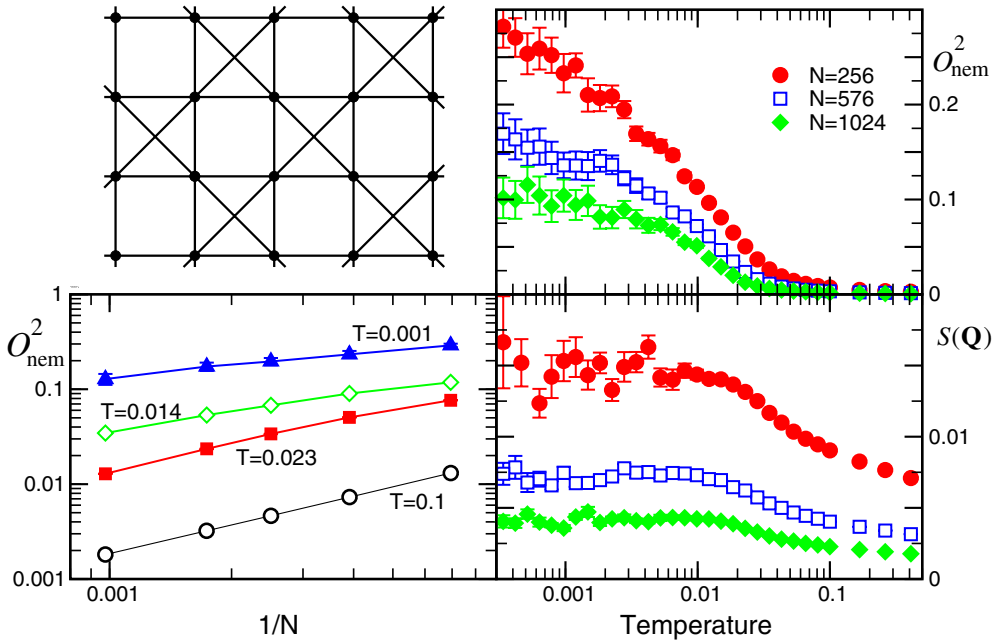

Figure 1. Top left panel: the checkerboard lattice. Two right panels: temperature dependences of squares of nematic (top) and Néel (bottom) order parameters for three lattice sizes. Left bottom panel: finite size scaling for the nematic order parameter. Temperatures are given in units of J.

where $\mathbf{S}_\mathrm{p} = \sum_{i\in p} \mathbf{S}_i$ is the total magnetization of a plaquette, N is the number of sites on the lattice and $N_\mathrm{p} = \frac{1}{2}N$ is the number of plaquettes. Minimizing the energy of a single plaquette, one obtains the classical constraint

$$\mathbf{S}_\mathrm{p} = \mathbf{H}/(2J). \tag{3}$$

The minimal total energy is reached if the above constraint is satisfied on every plaquette. In the field range $0 \leqslant H \leqslant H_\mathrm{sat} = 8J$ 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) various periodic and aperiodic spin structures are 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 a 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 ψ 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 $\psi^{\min}$ and the probability of finding 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 equation (2) is the same, $H_{\rm loc} = 2J$ for all sites and all external fields $0 \leqslant H \leqslant H_{\rm sat}$. The harmonic spin wave Hamiltonian is expressed as

$$\hat{\mathcal{H}}_2 = -H_{\rm loc} \sum_i S_i^x + J \sum_{\langle ij \rangle} S_i^y S_j^y \cos\theta_{ij}, \qquad S_i^x \approx 1 - \tfrac{1}{2} S_i^{y2}, \tag{4}$$

where components of every spin are taken in its local coordinate frame and θ_{ij} is an angle between neighbouring spins. The first term in $\hat{\mathcal{H}}_2$, which describes uncorrelated fluctuations of individual spins with $\langle S_i^{y2} \rangle = T/H_{\rm loc}$, 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 $\Delta F = -\langle \hat{V}^2 \rangle / 2T$:

$$\Delta F = -(T/8) \sum_{\langle ij \rangle} \cos^2\theta_{ij} = -(T/8) \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j)^2. \tag{5}$$

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 $\omega_{\mathbf{k}}^n$ and their contribution to the free energy:

$$\Delta F_2 = T \sum_n \sum_{\mathbf{k}} \ln(\omega_{\mathbf{k}}^n / \pi T). \tag{6}$$

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

An additional complication of highly frustrated magnets stems from the presence of several branches of zero modes: $\omega_{\mathbf{k}}^m \equiv 0$, in which case equation (6) is no longer correct. Instead, the low-T contribution to the free energy becomes

$$\Delta F = (N_2/2 + N_4/4) T \ln(J/T) + T \sum_{n \neq m, \mathbf{k}} \ln \omega_{\mathbf{k}}^n / J + T f_4, \tag{7}$$

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 the 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 configurations can be made on the 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 $\hat{\mathcal{H}}_2$ 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 [5–7]. Thus, the soft modes act similarly to harmonic excitations and stabilize collinear states. The presence of soft modes is most easily seen in the low-temperature specific heat, which is found from equation (7) to be $C = \frac{1}{2} - N_4/4N$. The deviation of the specific heat from a universal value of $C = \frac{1}{2}$ tells one how many soft modes exist in a low-temperature state of the XY checkerboard antiferromagnet.

3. Zero-field behaviour

At zero magnetic field the ground state constraint (3) specifies configurations with $\mathbf{S}_p = 0$ 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 $S_i^{y\text{down}} = -S_i^{y\text{down}}$ maps $\hat{\mathcal{H}}_2$ 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 the appearance of a quasi-long-range order at $\mathbf{q} = \mathbf{Q}$ when $T \to 0$. So-called weathervane defects [5] or wandering (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 $O_{\text{nem}}^{\alpha\beta} = \langle S_i^\alpha S_i^\beta \rangle - \frac{1}{2}\delta^{\alpha\beta}$ 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:

$$S(\mathbf{Q}) = \frac{1}{N^2}\sum_{i,j}\langle S_i^\alpha S_j^\alpha\rangle e^{i\mathbf{Q}(\mathbf{r}_i - \mathbf{r}_j)}, \qquad O_{\text{nem}}^2 = \frac{1}{N^2}\sum_{i,j}\langle S_i^\alpha S_i^\beta S_j^\alpha S_j^\beta\rangle - \frac{1}{2}. \quad (8)$$

The results are presented in figure 1. There is a clear signature of the nematic order seen from 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 Kosterlitz–Thouless 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 magnetization (3) are, generally, noncollinear, except for $H = \frac{1}{2}H_{\text{sat}}$, when a collinear 'uuud' state, figure 2(b), 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 figure 2. The first canted state, figure 2(a), exists in the whole range of fields and does not break the remaining spin reflection symmetry about the field direction. The second partially collinear state, figure 2(c), 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

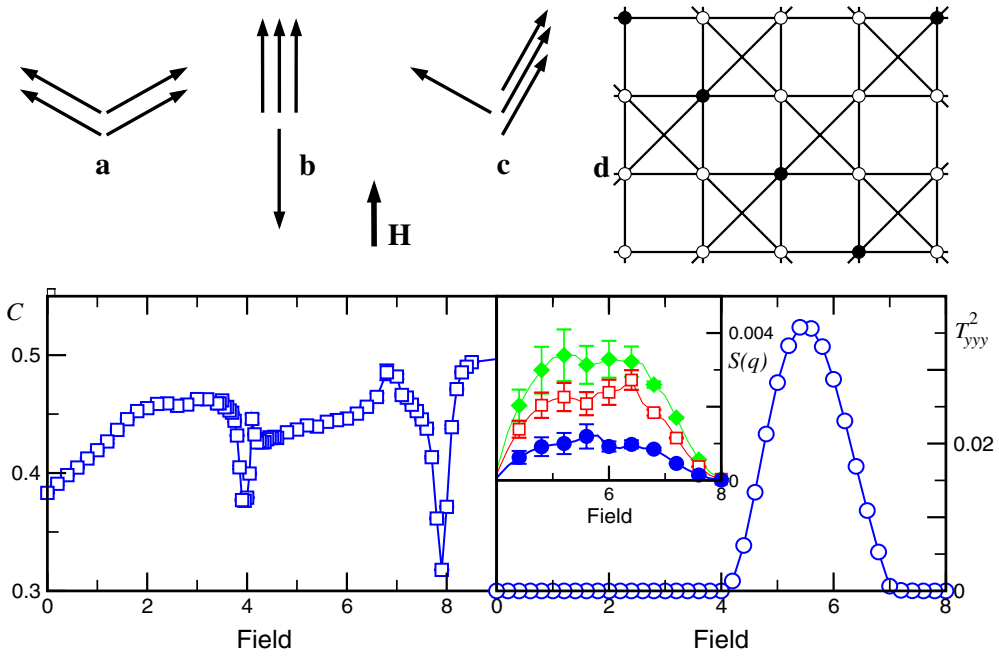

Figure 2. The top left panel shows three ground state configurations with maximal collinearity. The top right panel presents a translational pattern with the maximum number of soft modes for the partially collinear state (c). Bottom left panel: the field dependence of the specific heat for the $N = 1024$ cluster at $T = 0.002J$. Bottom right panel: the evolution of the triatic order parameter for the same cluster. The inset shows the field dependence of $S^{yy}(q)$ corresponding to state (d) for lattice sizes $N = 256$, 400, 1024 (from top to bottom). The magnetic field is given in units of J.

symmetry $\Delta F = -(T/8)[3 + \frac{1}{3}(8h^2 - 5)^2]$, $h = H/H_{\rm sat}$, over a 'less' collinear canted state $\Delta F = -(T/8)[2 + 4(2h^2 - 1)^2]$ 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 states 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 figure 2(d), 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 $T \geqslant 0.001J$ 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 $\langle S_i^y \rangle \equiv 0$, $\forall i$, in the high-field partially collinear state. Instead an Ising reflection symmetry is broken by a unique triatic order parameter:

$$T_{yyy} = \langle S_i^y S_i^y S_i^y \rangle. \tag{9}$$

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 figure 2 for $T = 0.002J$. C starts at a value which is very close to that analytically predicted $\frac{3}{8}$. In an applied field the system gradually loses soft modes up to $H = 0.5H_{\rm sat}$, where the 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 figure 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 data presented for $N = 1024$. The inset shows $S^{yy}(q)$ with $\mathbf{q} = (\pi, \pi)$ on a new lattice built from one sort of tetrahedra, which should be nonzero if the long-range order corresponding to figure 2(d) is present. The data obtained show that $S^{yy}(q) \equiv 0$ in the thermodynamic limit. Thus, the high-field state is described by the triatic order parameter T_{yyy}, which makes the checkerboard lattice 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 $\frac{1}{2}H_{\rm sat} < H < H_{\rm sat}$. Further theoretical investigations should focus on a unique H–T diagram of this model.

Acknowledgment

We thank the Theory Group of the Institute Laue-Langevin for use of their computer facilities for the current project.

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