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Thermodynamic and critical properties of an antiferromagnetically stacked triangular Ising antiferromagnet in a field

M. Žukovič *, M. Borovský, A. Bobák

Institute of Physics, Faculty of Science, P.J. Šafárik University, Park Angelinum 9, 040 01 Košice, Slovakia

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A B S T R A C T

We study a stacked triangular lattice Ising model with both intra- and inter-plane antiferromagnetic interactions in a field, by Monte Carlo simulation. We find only one phase transition from a paramagnetic to a partially disordered phase, which is of second order and 3D XY universality class. At low temperatures we identify two highly degenerate phases: at smaller (larger) fields the system shows long-range ordering in the stacking direction (within planes) but not in the planes (stacking direction). Nevertheless, crossovers to these phases do not have a character of conventional phase transitions but rather linear-chain-like excitations.

1. Introduction

A stacked triangular Ising antiferromagnet (STIA) is a geometrically frustrated spin system that has attracted considerable attention over the past several decades [1–21] due to its frustration-induced intriguing and controversial behavior as well as the fact that it reasonably describes some real magnetic materials, such as the spin-chain compounds $CsCoX_3$ (X is Cl or Br) and $Ca_3Co_2O_6$. The model consists of layers of triangular lattices stacked on top of each other thus forming linear chains of spins in the perpendicular direction. The interaction between spins within the chains (or between layers) can be considered to be either ferromagnetic (FSTIA model) or antiferromagnetic (ASTIA model). While the FSTIA model is relevant to the spin-chain compound $Ca_3Co_2O_6$ the ASTIA model can be used in modeling of $CsCoX_3$.

In the absence of an external magnetic field the physics of both systems is the same[1] and, therefore, most of the previous studies chose the FSTIA model for their investigations [1–7,10–15,18–21]. In zero field, the system has been found to undergo a second-order phase transition from the paramagnetic (P) to a partially disordered (PD) phase $(M,-M,0)$, with two sublattices ordered antiferromagnetically and the third one disordered. There is a wide consensus that the transition belongs to the 3D XY universality class [1,2,10,13,18] albeit the tricritical behavior has also been suggested [4]. Another phase transition at lower temperatures to a ferrimagnetic (FR) phase $(M,-M/2,-M/2)$, with one sublattice fully ordered and two partially disordered has been proposed [2,6,17] but questioned by several other studies [3,4,20,22], which argued that the low-temperature phase is a 3D analog of the 2D Wannier phase.

In the presence of the magnetic field, most of theoretical studies focused on elucidation of peculiar phenomena in magnetization processes observed in the experimental realization $Ca_3Co_2O_6$ [19,23–31]. Also critical properties of the FSTIA model have attracted a lot of interest due to phase transitions belonging to a variety of universality classes and multicritical behavior. In particular, the Monte-Carlo Mean-Field theory predicted the phase diagram in the temperature-field plane, with a small region of the PD phase stabilized at higher temperatures and small fields and the remaining part occupied by the FR phase [6]. The character of the P–PD transition line is concluded as second-order belonging to the XY universality class, however, at higher fields the P–FR transition line is identified as first-order due to its three-state Potts universality class. The FR–PD is reasoned to belong to the Ising universality class with possible crossover to the first-order behavior at low temperatures and very small fields. Later Monte Carlo simulations confirmed the first-order nature of the P–FR transition, however, suggested that the PD phase is probably destabilized by any finite field and phase transitions at smaller fields were determined to belong to the tricritical universality class [12].

* Corresponding author.
E-mail address: milan.zukovic@upjs.sk (M. Žukovič).

[1] The Hamiltonian of one model can be rewritten in terms of the other one with the spins in, e.g., odd layers inverted and the interlayer interaction sign changed, i.e., symbolically $H_A = J\sum(+1)(-1) = -J\sum(+1)(+1) = H_F$, where $J > 0$.

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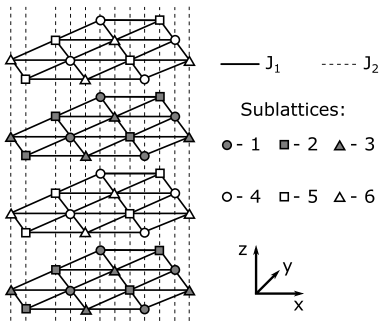

Fig. 1. ASTIA lattice partitioned into six sublattices marked by different symbols. The solid (dashed) lines represent intra-layer (inter-layer) interaction J_1 (J_2).

There have been attempts to also determine the phase diagram of the ASTIA model, which in the presence of the field is expected to differ from the FSTIA model, by the Monte-Carlo Mean-Field [7] and the Landau [8,9] theories. Both approaches predicted, besides the high-temperature P–PD line of second-order transitions, also one [7] and up to two [8,9] phase transitions to ferrimagnetic states at lower temperatures which can be first- or second-order of the Ising universality. The goal of the present study is to confront these early results obtained by the above approximate approaches with Monte Carlo (MC) simulations and a finite-size scaling analysis.

2. Model and methods

2.1. Model

We consider the ASTIA model described by the Hamiltonian

$$H = -J_1 \sum_{\langle i,j \rangle}^{xy} \sigma_i \sigma_j - J_2 \sum_{\langle i,k \rangle}^{z} \sigma_i \sigma_k - h \sum_i \sigma_i, \tag{1}$$

where $\sigma_i = \pm 1$ is an Ising spin variable, $J_1 < 0$ and $J_2 < 0$ are respectively antiferromagnetic intra-layer and inter-layer exchange interactions, h is an external magnetic field, and the first and second summations run over the nearest neighbor pairs within layers (in the xy plane) and between the layers (along the z axis), respectively. Due to the antiferromagnetic nature of both interactions J_1 and J_2 it is desirable to decompose the entire lattice into six interpenetrating sublattices, as shown in Fig. 1. The total coordination number is $z = 8$ and each spin is coupled to six neighbors from two sublattices $(3 + 3)$ in the same layer and two neighbors from another sublattice in the adjacent layers.

2.2. Monte Carlo simulations

In our Monte Carlo (MC) simulations we consider the ASTIA system of the size $V = L_x \times L_y \times L_z = L \times L \times 4L/3$, i.e., $L_z = 4L/3$ layers of the size $L \times L$ stacked along the z-axis, comprising in total $V = 4L^3/3$ spins. For obtaining temperature dependencies of various thermodynamic functions the linear lattice size is fixed to $L = 24$ and for the finite-size scaling (FSS) analysis it takes values $L = 24, 36$, and 48. In all simulations the periodic boundary conditions are imposed.

Initial spin states are randomly assigned and the updating follows the Metropolis dynamics. The lattice structure and the short range nature of the interactions enable vectorization of the algorithm. Since the spins on one sublattice interact only with the spins on the other, each sublattice can be updated simultaneously. Thus one sweep through the entire lattice involves just six sublattice updating steps. For thermal averaging, we typically consider $N = 10^5$ MC sweeps in the standard and up to $N = 10^7$ MC sweeps in the histogram MC simulations [32,33], after discarding another 20% of these numbers for thermalization. To assess uncertainty of the calculated quantities, we perform 10 runs, using different random initial configurations, and the error bars are taken as twice of the standard deviations.

We calculate the enthalpy per spin $e = E/V|J_1| = \langle H \rangle / V|J_1|$, where $\langle \cdots \rangle$ denotes the thermodynamic mean value, the sublattice magnetizations per spin

$$m_\alpha = 6\langle M_\alpha \rangle / V = 6\Big\langle \sum_{j \in \alpha} \sigma_j \Big\rangle / V, \ \alpha = 1, 2, \ldots, 6, \tag{2}$$

and the total magnetization per spin

$$m = \langle M \rangle / V = \Big\langle \sum_{i=1}^{V} \sigma_i \Big\rangle / V. \tag{3}$$

The magnetic susceptibility is defined as

$$\chi_m = \beta(\langle M^2 \rangle - \langle M \rangle^2)/V, \tag{4}$$

and the specific heat as

$$C = \beta^2(\langle E^2 \rangle - \langle E \rangle^2)/V, \tag{5}$$

where $\beta = 1/k_B T$. To measure a degree of the ferrimagnetic ordering within the planes and the antiferromagnetic ordering in the stacking direction, we introduce the order parameters o_{xy} and o_z, defined as

$$o_{xy} = \langle O_{xy} \rangle_z / L^2 = \langle M_{max} - M_{min} + |M_{med}| \rangle_z / L^2, \tag{6}$$

and

$$o_z = \langle O_z \rangle / L_z = \Big\langle \sum_{k=1}^{L_z} (-1)^k \sigma_k \Big\rangle_{xy} / L_z, \tag{7}$$

where M_{max}, M_{min}, and M_{med} are sublattice magnetizations in each plane with the maximum, minimum, and medium (remaining) values, respectively, and the symbols $\langle \cdots \rangle_z$ and $\langle \cdots \rangle_{xy}$ denote the mean values taken over the planes and over the chains, respectively.

To study phase transitions in the present six-sublattice system, we define the order parameter in accordance with Ref. [34] as

$$o = \langle O \rangle / V = \left\langle \frac{\sqrt{3}}{3} \left(\sum_{\alpha=1}^{6} O_\alpha^2 \right)^{1/2} \right\rangle \Big/ V, \tag{8}$$

where $O_1 = (M_1 - (M_2 + M_3)/2)/2$, $O_2 = (M_2 - (M_1 + M_3)/2)/2$, $O_3 = (M_3 - (M_1 + M_2)/2)/2$, $O_4 = (O_4 - (M_5 + M_6)/2)/2$, $O_5 = (M_5 - (M_4 + M_6)/2)/2$, $O_6 = (M_6 - (M_4 + M_5)/2)/2$, and the corresponding susceptibility

$$\chi_o = \beta(\langle O^2 \rangle - \langle O \rangle^2)/V. \tag{9}$$

In order to calculate the critical exponents and thus determine the order of the transition and also the universality class if the transition is second order, we employ a FSS analysis with the following scaling relations:

$$C(L) \propto L^{\alpha/\nu}, \tag{10}$$

$$O(L) \propto L^{-\beta/\nu}, \tag{11}$$

$$\chi(L) \propto L^{\gamma/\nu}, \tag{12}$$

$$\frac{d\langle O \rangle}{d\beta} = \langle O \rangle \langle E \rangle - \langle O E \rangle \propto L^{(1-\beta)/\nu}, \tag{13}$$

$$\frac{d \ln \langle O^2 \rangle}{d\beta} = \langle E \rangle - \frac{\langle O^2 E \rangle}{\langle O^2 \rangle} \propto L^{1/\nu}, \tag{14}$$