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Physica A 275 (2000) 207–216

PHYSICA A

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First-order transition in helimagnetic systems with Heisenberg spins

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Received 25 May 1999

Abstract

We perform Monte Carlo simulations on the body-centered-tetragonal helimagnet with Heisenberg spins which has the same breakdown of symmetry as the stacked triangular antiferromagnetic lattices and must belong to the same universality class. We obtain a second-order transition with similar critical exponents showing slight differences, which may be connected to the effects of the periodic boundary conditions imposed on MC simulations. This is in contradiction with the renormalization group (RG) studies which predict a first-order transition. Using Zumbach's concept of a complex fixed point we reconcile the difference in behavior between simulation and RG studies and show that the transition should be of first order for an infinite system. © 2000 Elsevier Science B.V. All rights reserved.

PACS: 05.70.Fh; 64.60.Cn; 75.10.-b

Keywords: Phase transition; Monte Carlo; Frustrated spins system

1. Introduction

Phase transitions in frustrated Heisenberg spin systems have been studied extensively during the last decade (for reviews see Ref. [1]). In particular, when the ground state is non-collinear (but planar) and therefore the $SO(3)$ symmetry group at high temperatures is completely broken at low-temperatures. This situation is different from the breakdown for non frustrated systems where the symmetry group in the low-temperature region is $SO(2)$. The difference in the breakdown of symmetry between frustrated and non-frustrated spin systems should lead to different critical behavior. The RG studies

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PII : S0378-4371(99)00360-X

Table 1
Critical exponents by Monte Carlo[a] and by RG[b] for $SO(3)$

Systems	Ref.	α	β	γ	ν	η
STA[a]	[7]	0.240(80)	0.300(20)	1.170(70)	0.590(20)	+0.020(180)[c]
STA[a]	[8]	0.242(24)[d]	0.285(11)	1.185(3)	0.586(8)	−0.033(19)[c]
STA[a]	[9]	0.245(27)[d]	0.289(15)	1.176(26)	0.585(9)	−0.011(14)[c]
STA[a]	[10]	0.230(30)[d]	0.280(15)		0.590(10)	0.000(40)[e]
Bct[a]	This work	0.287(30)[d]	0.247(10)	1.217(32)	0.571(10)	−0.131(18)[c]
Ferro.[b]	[29]	−0.117	0.366	1.386	0.706	0.038*

*Notes: STA = stacked triangular antiferromagnetic; Bct = body-centered-tetragonal; [c] Calculated by $\gamma/\nu = 2 - \eta$; [d] Calculated by $d\nu = 2 - \alpha$; [e] Calculated by $2\beta/\nu = d - 2 + \eta$.

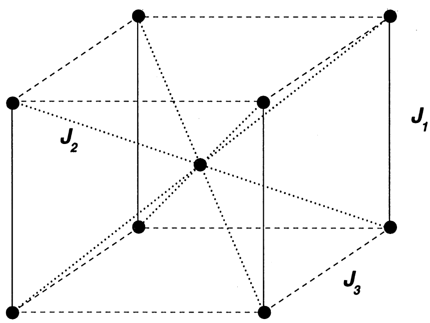

Fig. 1. The body-centered tetragonal lattice cell.

have been carried out by Bailin et al. [2], Garel et al. [3] and Kawamura [4,5] in two loop and Antonenko et al. [6,7] in three loop approximation. These last authors have found, after Pade–Borel resummation, that the transition is of second order if the number of components of the spins N is more than $N_c = 3.91$ and first order if N is less than N_c. Thus for Heisenberg spins ($N = 3 < N_c$) the transition should be first order. This is in contradiction with the results of numerous Monte Carlo (MC) simulations on STA [8–13] which give results different from the standard $O(N)$ ferromagnetic universality class (Table 1) and favor a new *chiral* universality class as proposed by Kawamura [4]. For more discussion about this question see Refs. [14,15].

In this article we studied the body-centered-tetragonal (bct) helimagnets which have the same breakdown of symmetry as the STA and should therefore belong to the same universality class. The bct lattice, shown in Fig. 1, is similar to the helimagnetic order found experimentally in holmium (Ho), dysprosium (Dy) and terbium (Tb). However, these compounds have a strong XY anisotropy and do not correspond exactly to our model (for a review see Ref. [14]). The model we study has been investigated with MC simulations by Diep [16] but the results were not very conclusive (see discussion in section results) and only the exponent ν has been found. With greater sizes and better statistics we obtain a clear second-order transition with exponents compatible with those found in STA (see Table 1) thus in favor of a new universality class and in contradiction with the RG studies. However, using Zumbach's concept of a complex

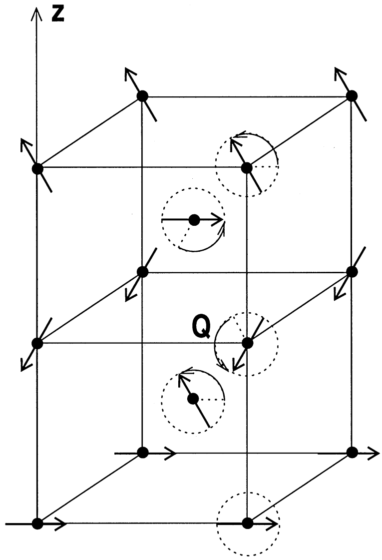

Fig. 2. Ground state configuration for $J_2/J_1 = 0.5$ and $Q = 120^{\circ}$.

fixed point [15,17,18] we will be able to reconciliate the results of simulations and RG studies. In particular, we show that the second-order transition obtained in MC simulations is due to a fixed point in the complex parameter space which has a strong influence on the real parameter space and forces the systems with finite size to mimic a second-order transition.

Our work is organized as follows. In Section 2 we present the model and the MC procedure. The thermodynamic quantities, their finite size scaling behavior and the methods to calculate the critical exponents are exposed in Section 3. The results are shown and discussed in Section 4 and Section 5 is devoted to the conclusion.

2. Model and simulation

We study for the classical $O(3)$ spins on a bct lattice. The Hamiltonian is given by

$$H = J_1 \sum_{(ij)} \mathbf{S}_i.\mathbf{S}_j + J_2 \sum_{(ij)} \mathbf{S}_i.\mathbf{S}_j + J_3 \sum_{(ij)} \mathbf{S}_i.\mathbf{S}_j \,, \tag{1}$$

where $\mathbf{S}_i$ are the three component classical vectors of unit length and the three sums represent the nearest neighbors in different directions (see Fig. 1). We choose $J_3 = 0$. The competition between antiferromagnetic interactions J_1 and J_2 gives rise to a helical ordering along the z-axis at $T = 0$ (see Fig. 2). This ground state is defined by Q the turn angle between spins belonging to two adjacent planes perpendicular to the z-axis. Minimizing (1) leads to the value of Q:

$$\cos(Q) = -\frac{J_2}{J_1} \,. \tag{2}$$

In this article we will use the ratio $J_2/J_1 = 0.5$ thus, Q will be equal to 120° as in STA. It is obvious that the exact value of the turn angle is an irrelevant parameter for the critical behavior [19]. Indeed all systems with a planar ground state will belong to the same universality class. However this value must be commensurate with the lattice periodicity because we impose periodic conditions in our simulations. The reader interested in the complete phase diagram when J_2/J_1 varies between 0 and ∞ should consult Refs. [16,20].

The MC updating procedure is the standard Metropolis algorithm to update one spin after the other. In each simulation 1 million of MC step updatings were carried out for equilibration and up to 5 million of MC steps for the largest sizes were made to obtain averages. We consider $L(L/2)^2$ systems, where $(L/2)^2$ is the size of the planes, and L is the number of planes in the z-axis. L must be a multiple of two for a bct lattice and also a multiple of three so that no frustration occurs because of periodic boundary conditions along the z-axis. Simulations have been done for system sizes with $L = 18$, 24, 30, 36, 42, 54, 60.

The order parameter M for this model is

$$M = \frac{1}{L}\sum_{i=1}^{L} |M_i| \,, \tag{3}$$

where M_i $(i = 1,\ldots,L)$ is the magnetization for each plane.

We use in this work the MC histogram technique developed by Ferrenberg and Swendsen [21,22]. From a simulation done at T_0, this technique allows to obtain thermodynamic quantities for T close to T_0. Since the energy spectrum of a Heisenberg spin system is continuous, the choice of the bin size for the histogram must be made. In order to use the histogram method efficiently, it is sufficient to divide the energy range into 30,000 intervals (we have verified that we obtain the same results with our statistical precision for 100,000 intervals).

Our errors are calculated with the help of the Jackknife procedure [23].

3. Finite size scaling

The quantities needed for our analysis in the FSS region are defined below. For each temperature we calculate

$$C = \frac{\langle E^2\rangle - \langle E\rangle^2}{Nk_BT^2} \,, \tag{4}$$

$$\chi = \frac{N(\langle M^2\rangle - \langle M\rangle^2)}{k_BT} \,, \tag{5}$$

$$\chi_2 = \frac{N\langle M^2\rangle}{k_BT} \,, \tag{6}$$

$$V_1 = \frac{\langle ME\rangle}{\langle M\rangle} - \langle E\rangle \,, \tag{7}$$

$$V_2 = \frac{\langle M^2 E\rangle}{\langle M^2\rangle} - \langle E\rangle \,, \tag{8}$$

$$U = 1 - \frac{\langle M^4\rangle}{3\langle M^2\rangle^2} \,, \tag{9}$$

where T is the temperature, M the order parameter, C the specific heat per site, χ the magnetic susceptibility per site, χ_2 the magnetic susceptibility per site in the high-temperature region where the order parameter is zero, V_1 and V_2 are cumulants which we use to obtain the critical exponent v, U the fourth-order cumulant, $\langle\cdots\rangle$ means the thermal average.

According to the FSS theory [24,25] for a second-order transition, the various quantities just defined should scale for a sufficiently large system at the critical temperature T_c like:

$$\chi = L^{\gamma/v} g_\chi \,, \tag{10}$$

$$\chi_2 = L^{\gamma/v} g_{\chi_2} \,, \tag{11}$$

$$V_1 = L^{1/v} g_{V_1} \,, \tag{12}$$

$$V_2 = L^{1/v} g_{V_2} \,, \tag{13}$$

$$\langle M\rangle = L^{-\beta/v} g_M \,, \tag{14}$$

where g are the constants independent of size L.

To find T_c we use U. We record the variation of U with T for various system sizes and then locate the intersection of these curves. We compare the value of U for two different lattice sizes L and $L' = bL$, making use of the condition [26]

$$\left.\frac{U_{bL}}{U_L}\right|_{T=T_c} = 1. \tag{15}$$

Due to the presence of residual corrections to finite size scaling, one actually has to extrapolate the results taking the limit $(\ln b)^{-1} \to 0$ (Figs. 3 and 4).

4. Results

We first determine T_c using (15). In Fig. 3, U is plotted as the function of the temperature for different sizes from L=18 to 60. From this data and (15) we extrapolate the value of T_c in Fig. 4 and obtain

$$T_c = 1.05105(15) \,. \tag{16}$$

We estimate the universal quantity U at T_c (U^*)

$$U^* = 0.639(1) \,. \tag{17}$$

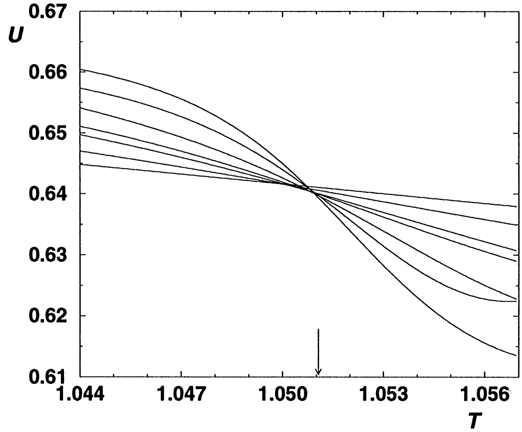

Fig. 3. Binder's parameter U as a function of the temperature for different sizes L (in the left part of the figure, from $L = 18$ (down) to $L = 60$ (up). The arrow shows the estimated critical temperature T_c.

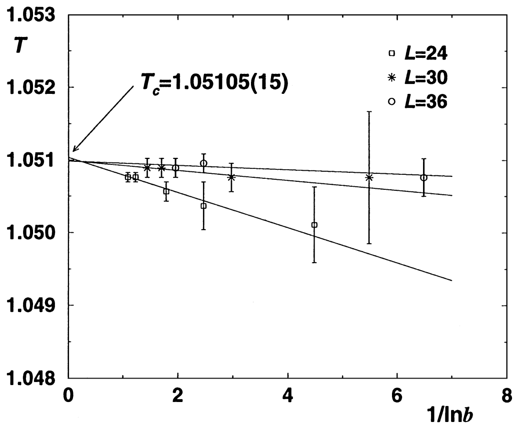

Fig. 4. Estimated T_c plotted vs. inverse logarithm of the scale factor $b = L'/L$. For clarity, only the results for $L = 24, 30, 36$ are shown. The estimated temperature is $T_c = 1.05105(15)$.

With the value of T_c (16) we find the critical exponents by log–log fits. We obtain from V_1 and V_2 (Fig. 5), from χ and χ_2 (Fig. 6) and from $\langle M \rangle$ (Fig. 7)

$$\nu = 0.570(10)\,, \tag{18}$$

$$\nu = 0.571(10)\,, \tag{19}$$

$$\frac{\gamma}{\nu} = 2.132(20)\,, \tag{20}$$

$$\frac{\gamma}{\nu} = 2.130(18)\,, \tag{21}$$

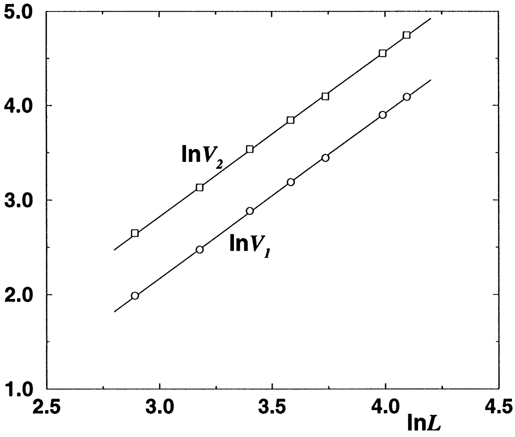

Fig. 5. Value of V_1 and V_2 as a function of L in an ln–ln scale at T_c. The value of the slopes gives $1/\nu$ and we obtain $\nu = 0.570(10)$ and 0.571(10), respectively. The size $L = 18$ is not included in the fit. The estimated error bars are smaller than the symbols.

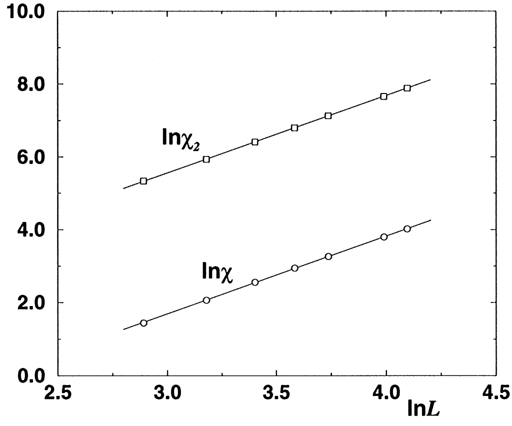

Fig. 6. Value of χ and χ_2 as a function of L in an ln–ln scale at T_c. The value of the slope gives γ/ν. We obtain 2.132(20) and 2.130(18), respectively. The size $L = 18$ is not included in the fit. The estimated error bars are smaller than the symbols.

$$\frac{\beta}{\nu} = 0.432(10)\,, \tag{22}$$

respectively. The errors include the influence of the uncertainty in the estimate of T_c. We obtain with these values, $\beta = 0.247(10)$ and $\gamma = 1.217(32)$. We calculate η from the scaling relation

$$\frac{\gamma}{\nu} = 2 - \eta \tag{23}$$

and obtain $\eta = -0.131(18)$ (Our results are summarized in Table 1).

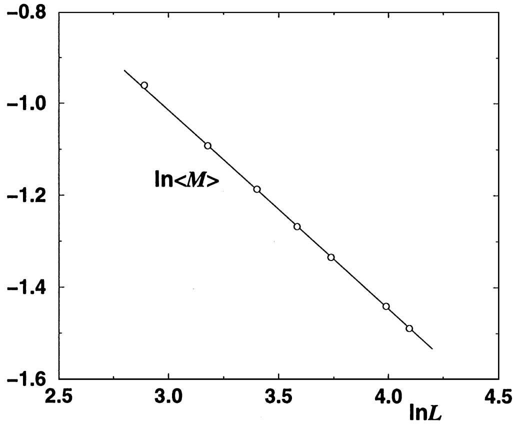

Fig. 7. Value of $\langle M\rangle$ as a function of L in an ln–ln scale at T_c. The value of the slopes gives β/ν and we obtain 0.432(10). The size $L=18$ is not included in the fit. The estimated error bars are smaller than the symbols.

The negative value of η is obviously impossible because it should always be positive [15,27,28]. This has been used by us before [14] as a criterion to decide whether the transition is caused by a fixed point in the complex plane. However the value of η is much more negative if we compare it with the values found in simulations on STA (see Table 1) and we think that it is due to the incompatibility between the periodic boundary conditions and the turn angle Q. Indeed it has been shown that Q can vary as a function of the temperature, for example, in experimental studies of helimagnets [29,30], with a mean field approximation [31] or with MC simulations on different systems [32]. Thus the lattice size L which is commensurate with Q at $T=0$ is not at T_c. This implies more frustration and can make the critical exponents vary from their original values. This is surely the explanation why Diep [16] obtained a first-order transition for XY spins on the bct lattices whereas the results on STA give a second-order transition (see a review in Ref. [14]).

We compare now our study with Diep for Heisenberg spins [16]. He obtained the results concerning T_c and ν using the FSS relation $T_c(L)=T_c+aL^{-1/\nu}$ at which $T_c(L)$ is the temperature where the specific heat of each size L is maximum. If we use a fit procedure with three unknown parameters [33] for his results ($T_c(12)=1.000(5)$, $T_c(18)=1.025(5)$, $T_c(24)=1.0350(25)$, $T_c(30)=1.0400(25)$, $T_c(36)=1.0425(25)$, $T_c(42)=1.0440(25)$) we obtain: $T_c=1.0495(61)$, $\nu=0.56(19)$, $a=-4.(6)$. These values are in agreement with our results but we use better statistics and bigger sizes, therefore our results are more accurate. This is to be expected since it has been proved in numerous MC that the specific heat results are very unstable and will not give reliable results for critical exponents (for example see Ref. [34]).

5. Conclusion

We have obtained results for a canted spin structure on a bct lattice compatible with the results found with simulations on the stacked triangular lattice (STA) which agree also with the experimental studies (see review in Ref. [15]). The values of the critical exponents are different from those of the standard universality class and are in favor of a new *chiral* universality class [4,5]. However, they are in contradiction with the first-order behavior predicted by the RG studies [6,7]. We will explain now how we can reconcile the different methods (the reader can consult also Ref. [15] for more details). The RG predicts that a stable fixed point F_+ if $N > N_C = 3.91$ exists in three dimensions corresponding to a new universality class (the *chiral* class of Kawamura). When $N < N_c$ the solution of equations become complex, thus there is no longer a stable fixed point and this absence is interpreted as a first-order transition. But, as remarked by Zumbach [17,18], a *complex fixed point*, or minimum in the flow, emerges and can have a strong influence on the real plane parameters if it is close to the real axis and if it has a large basin of attraction. The transition appears to be first order only when the system is very large, that is if $L > \xi_0$ where ξ_0 is the largest correlation length in the basin of attraction of F_+. If $L < \xi_0$ the system stays under the influence of the complex fixed point.

So we conclude that the transition in helimagnetic systems with Heisenberg spins is of first order but due to the finite size used in numerical simulations the systems mimic a second-order transition due to a complex fixed point. Moreover, problems in periodic conditions in MC lead to corrections in the values of the critical exponents.

Acknowledgements

This work was supported by the Alexander von Humboldt Foundation. We are grateful to Professors K.D. Schotte, G. Zumbach, B. Delamotte, H.T. Diep and A. Dobry for discussions. We thank A.I. Sokolov and E. Brezin for the reference of the proof of $\eta \geqslant 0$.

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