Physica A 388 (2009) 1111–1119

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Percolation properties of the antiferromagnetic Blume–Capel model in the presence of a magnetic field

G. Pawłowski

Faculty of Physics, A. Mickiewicz University, Umultowska 85, 61-614 Poznań, Poland

ARTICLE INFO

Article history:
Received 13 February 2008
Received in revised form 16 December 2008
Available online 7 January 2009

PACS:
05.50.+q
64.60.-i
64.60.Cn
02.70.Rr

Keywords:
Phase transitions
Percolation problem
Blume–Capel model

ABSTRACT

The problem of order–order and order–disorder transitions in the system described by the 2D antiferromagnetic Blume–Capel model in the presence of a magnetic field is studied by the Wang and Landau flat-histogram simulation method and by the classical Monte Carlo. Anomalous thermodynamic characteristics in low temperatures indicate different type orderings in finite temperatures. The existence of pure antiferromagnetic phases as well as mixed state is shown by detailed phenomenological analysis of the system. The border lines on the phase diagram between various orderings are determined by the complementary microscopic study of the percolation problem for $c(2 \times 2)$ elementary structures of antiferromagnetic ordered phases. This new approach has also shown a full agreement between the percolation threshold for the cluster of mixed phase and the critical temperature of the ordered system.

1. Introduction

The subject of the study is the classical spin-1 system with single-ion anisotropy in the presence of a magnetic field, known in literature as the Blume–Capel (BC) model [1]. The Hamiltonian of the model is given by

$$\mathcal{H} = -J \sum_{i,j} S_i S_j + D \sum_i S_i^2 - H \sum_i S_i, \tag{1}$$

where S_i is the spin-1 Ising operator, J is the spin–spin interaction between nearest-neighbours, D is the single-ion anisotropy and H is the external magnetic field. The model has been thoroughly studied for different lattices by many analytical and simulation methods, e.g. Refs. [2–6]. The rich critical behaviour is accompanied by existence or mixing of different ordered phases (Fig. 1). In this paper we have focused on the latter problem, which has been relatively little studied.

The first method of the investigation is that of the flat histogram, known also as the Wang–Landau (WL) sampling method [7], that has been applied to a wide class of classical and quantum models [8–10]. The calculations for BC model by the WL method have been presented in a short paper by the author [11] for the antiferromagnetic case. A detailed analysis for the ferromagnetic case has been made by Silva, Caparica and Plascak [12].

The model analyzed is characterised by a considerable complexity of phase diagrams. In the antiferromagnetic case ($J < 0$) and in the presence of magnetic field in the ground state (GS) we observe two kinds of ordered phases (Fig. 1): for small values of H there exists the Ising $S = 1(1, -1)$ antiferromagnetic phase, which we call in this paper AF1, but for higher values of the magnetic field we can also observe the second antiferromagnetic phase $(0, \pm 1)$ (respectively for $H > 0$ or $H < 0$, which we call here AF2). In the ground state there is a discontinuous order–order transition (described by the equation $|H| = 4|J| - D$ for $0 \leq D/|J| \leq 2$).

E-mail address: gpawlo@amu.edu.pl.

0378-4371/$ – see front matter © 2009 Elsevier B.V. All rights reserved.
doi:10.1016/j.physa.2008.12.057

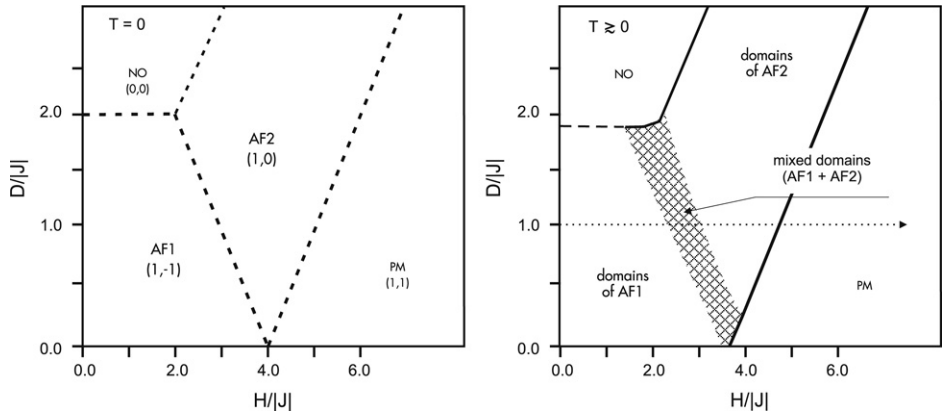

Fig. 1. The phase diagram of the antiferromagnetic Blume–Capel model in the presence of a magnetic field in the extrapolated ground state and in low temperatures. The solid and the dashed lines indicate the second and the first order transitions, respectively. The dotted line presents the main direction of the currently analysis at finite temperatures. Denotations: AF1 and AF2 — antiferromagnetic phases, NO — nonordered (nonmagnetic) phase and PM — paramagnetic phase.

The paper reports accurate calculations of density of states (DOS) in the ranges of the first and second order phase transitions and determination of the thermodynamical quantities such as internal energy, free energy, specific heat and entropy. Then, on the basis of a standard analysis of singularities in the thermodynamical characteristics the phase transition points have been established. Although the analysis has been made for the whole range of the model parameters, detailed results are presented for selected values of magnetic field for the case of $D/|J| = 1.0$ (Sections 2 and 3).

Here we have applied the WL method to a 2D square lattice with periodic boundary conditions for a relatively small system $L = 20$. The analogous analysis for bigger system is more difficult and must be longer in order to take a walk over the whole larger energy space many times. Although the procedure converged for any large L, the results of DOS are very incoherent for too short computer times, when the measured flatness is too weak. For presented results the modification factor changes from $f_0 = e$ to the final factor $\ln(f) \approx 10^{-9}$. The flatness criterion was put on 95% level. The average values obtained after many cycles of simulation for the same model parameters are taken for future calculations. The resulting precision of the WL method is very high as the relative error of different series varies in the range 10^{-3}–10^{-4}.

Our new and highly accurate measurements by the WL method have shown that in finite temperatures the AF1–AF2 transition is decomposed into two branches separating the pure phases by a mixed state, so that three distinct ordered areas appear (Fig. 1). The temperature dependencies of specific heat, internal energy and entropy reveal anomalies in finite temperatures and as shown by the cluster analysis (Section 3) though they are not a consequence of the finite-size of the system but of realible different ordering of the system. The very identification of these anomalies has brought the advantage of a correct description of different ordered states of the antiferromagnetic BC model at finite temperatures.

In Section 3 we have performed standard Monte Carlo simulations to search for the *spanning clusters* of AF1 and AF2 elementary cells $c(2 \times 2)$. It is significant that the problem of order–order transition can also be described in terms of the percolation theory. The analysis presented is a continuation of what has been done in Ref. [11] for pure phases. The main point of this paper is the accurate percolation analysis for a mixed state in a wide range of the model parameters. Apart from confirming the thesis of existence of a third separate region of ordering, the results obtained have revealed a full agreement between the percolation thresholds in the thermodynamical limit with the critical temperatures of the ordered system. The accuracy of the coincidence of the results was of the order of the very high accuracy of the methods used. For different lattice sizes of the system $L = 10$–100, the lengths of the MC simulations varied from 5000 to 450 000 MCS, where we discarded about 10% for lattice thermalization. The error was estimated by a standard binning method [13]. Since the critical behaviour was analyzed in the region of continuous transition, the errors were very small and the bars were omitted on the plots. The cluster analysis was done for any accepted sample using enhanced Hoshen–Kopelman algorithm [14] for *reduced binary lattices* (the site percolation problem) defined separately for *any* possible orders present in the system [15].

Both WL and classical MC methods are complementary and give compatible results. The analysis based on the accurate DOS calculation gives a complete phenomenological description, which allows explanation of the physical nature of the phase transitions observed, while the classical MC enables additionally microscopic view on a cluster present in the system in given thermodynamic conditions. As the coincidence between both methods is well visible, the results give a new alternative interpretation of phase transitions in the antiferromagnetic BC model in a magnetic field.

2. Results of Wang–Landau sampling method

To analyze thermodynamic properties of a system we have used the simulation method, in which the density of states $g(E)$ is highly accurately determined by sampling in the space of energy. This method is based on the idea of the flat histogram, built during a random walk in the energy space with a probability proportional to the reciprocal of the density of