Physica A 389 (2010) 5402–5407

Contents lists available at ScienceDirect

Physica A

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

Phase diagram of a mixed spin-1 and spin-3/2 Ising ferrimagnet

M. Žukovič *, A. Bobák

Department of Theoretical Physics and Astrophysics, Faculty of Science, P.J. Šafárik University, Park Angelinum 9, 041 54 Košice, Slovak Republic

ARTICLE INFO

Article history:
Received 7 July 2010
Received in revised form 10 August 2010
Available online 18 August 2010

Keywords:
Ferrimagnet
Mixed-spin system
Phase diagram
Ising model
Monte Carlo simulation
Compensation temperature

ABSTRACT

Critical and compensation properties of a mixed spin-1 and spin-3/2 Ising ferrimagnet on a square lattice are investigated by standard and histogram Monte Carlo simulations. The critical temperature is studied as a function of single-ion anisotropy strength. The second order of the phase transition is established by finite-size scaling for the entire boundary. Some previously obtained results, such as a tricritical point, predicted by the mean field theory (MFT) and the effective field theory (EFT), or a first-order transition line separating two different ordered phases, obtained by the cluster variational theory (CVT), are deemed artifacts of the respective approximations. So is a re-entrant phenomenon produced by CVT. Nevertheless, the multicompensation behavior predicted by MFT and EFT was confirmed.

1. Introduction

There have been a number of theoretical studies of mixed-spin Ising ferrimagnets as simple models of certain types of molecular-based magnetic materials [1–5]. Besides other interesting properties, such as the appearance of multicritical behavior, they attract attention due to the so-called compensation behavior with possible technological applications. Such a phenomenon occurs at a compensation temperature, i.e., the temperature below the critical point at which the sublattice magnetizations completely cancel out and the total magnetization changes sign. Generally speaking, from the previous studies it can be concluded that the higher values of spins and the more complex lattice topologies used, the richer behavior can be expected. However, the increasing complexity usually requires increasing simplifications in the approaches for the problem to be manageable. Thus nonperturbative approaches, such as exact [6–10] and Monte Carlo (MC) [11–14], are so far limited to the simplest cases of either the smallest spin values (i.e., mixed spin-1/2 and spin-1) or the lattice topology (e.g., honeycomb or Bethe lattices). As a consequence, the behavior of the mixed spin-1/2 and spin-1 Ising system is rather well understood, while there are still disagreements among different theoretical investigations of the mixed-spin systems with higher spin values, including the spin-1 and spin-3/2 case. The disagreements arise from the fact that due to higher complexity, mostly different approximative schemes with various degrees of approximation have been employed, such as the mean field theory (MFT) [15], the effective field theory (EFT) [16–18] and the cluster variational theory (CVT) [19]. These approximative approaches have been previously shown to produce some artifacts, such as a tricritical point, predicted by MFT [20] and EFT [21] for the mixed spin-1/2 and spin-1 system on a square lattice, that were not reproduced either in numerical transfer matrix [12] or MC studies [11,12,14]. To our knowledge, the results of these approximative studies for the mixed spin-1 and spin-3/2 system have so far been verified by MC simulations only for the case of a simple cubic lattice [22]. However, for this particular case, there were basically no qualitative disagreements among the conclusions drawn from the respective studies and the MC results only confirmed the previously obtained results. On the other hand, for the cases of honeycomb and square lattices, there are qualitative differences in the results, which have not been resolved yet.

* Corresponding author.
E-mail addresses: milan.zukovic@upjs.sk (M. Žukovič), andrej.bobak@upjs.sk (A. Bobák).

0378-4371/$ – see front matter
doi:10.1016/j.physa.2010.08.012

The objective of this study is to focus on the case of the mixed spin-1 and spin-3/2 Ising system with uniform single-ion anisotropy on a square lattice, for which the differences between the MFT, EFT and CVT results are the most prominent. In particular, we aim to answer the following questions: (1) Are the phase transitions of second order for the entire range of the anisotropy strength, as predicted by CVT, or is there a tricritical point separating lines of the second- and first-order transitions, as predicted by both MFT and EFT? (2) Is there a re-entrant phenomenon in the second-order phase boundary, as suggested by the CVT results but not by MFT nor EFT? (3) Does the line of first-order transitions situated within the ordered ferrimagnetic region, obtained by CVT but not by MFT nor EFT, really exist? (4) Can the system display up to two compensation points, as predicted by both MFT and EFT (not investigated by CVT)?

2. Model and Monte Carlo simulations

The model of the mixed spin-1 and spin-3/2 Ising system on the square lattice is described by the Hamiltonian

$$H = -J \sum_{(i,j)} S_i^A S_j^B - D_A \sum_i (S_i^A)^2 - D_B \sum_j (S_j^B)^2, \tag{1}$$

where $S_i^A = \pm\frac{3}{2}, \pm\frac{1}{2}$ for A ions, $S_j^B = \pm 1, 0$ for B ions, $J < 0$ is the nearest-neighbor coupling parameter between the ions on A and B sublattices, and D_A, D_B are the single-ion anisotropies acting on the spin-3/2 and spin-1 ions, respectively. In this study we will consider the anisotropy of uniform strength, i.e., $D \equiv D_A = D_B$.

A simulated $L \times L$ square lattice consists of two interpenetrating sublattices, each one comprising $L^2/2$ sites. We consider linear lattice sizes ranging from $L = 20$ up to $L = 200$ with the periodic boundary conditions imposed. Initial spin states are randomly assigned and the updating follows the Metropolis dynamics. The lattice structure and the short range 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 two 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 [23,24], after discarding another 20% of these numbers for thermalization. To assess uncertainty, we perform ten runs, using different random initial configurations. Then the errors of the calculated quantities are determined from the values obtained for those runs as twice the standard deviations.

We calculate the internal energy per site $e = E/L^2 = \langle H \rangle / L^2$ and the sublattice magnetizations per site

$$m_A = 2\langle M_A \rangle / L^2 = 2 \left\langle \left| \sum_A S_i^A \right| \right\rangle \Big/ L^2, \tag{2}$$

$$m_B = 2\langle M_B \rangle / L^2 = 2 \left\langle - \left| \sum_B S_j^B \right| \right\rangle \Big/ L^2, \tag{3}$$

where $\langle \cdots \rangle$ denotes thermal averages. The total magnetization per site is defined as

$$m = \langle M \rangle / L^2 = \langle M_A + M_B \rangle / L^2. \tag{4}$$

Since for ferrimagnets m can vanish within the ordered phase at the compensation temperature, as an order parameter it is useful to define the staggered magnetization per site as

$$m_s = \langle M_s \rangle / L^2 = \langle M_A - M_B \rangle / L^2. \tag{5}$$

Further, the following quantities which are functions of the parameters E or/and $O(= M,\ M_s)$ are defined: the specific heat per site c

$$c = \frac{\langle E^2 \rangle - \langle E \rangle^2}{L^2 k_B T^2}, \tag{6}$$

the direct ($O = M$) and staggered ($O = M_s$) susceptibilities per site χ_O

$$\chi_O = \frac{\langle O^2 \rangle - \langle O \rangle^2}{L^2 k_B T}, \tag{7}$$

the logarithmic derivatives of $\langle O \rangle$ and $\langle O^2 \rangle$ with respect to $\beta = 1/k_B T$

$$D_{1O} = \frac{\partial}{\partial \beta} \ln\langle O \rangle = \frac{\langle OE \rangle}{\langle O \rangle} - \langle E \rangle, \tag{8}$$

$$D_{2O} = \frac{\partial}{\partial \beta} \ln\langle O^2 \rangle = \frac{\langle O^2 E \rangle}{\langle O^2 \rangle} - \langle E \rangle, \tag{9}$$