Phase Diagram of the Antiferromagnetic Blume-Capel Model on Triangular Lattice

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Abstract. We perform Monte-Carlo simulations of the anti-ferromagnetic (AF) spin-1 Blume-Capel (BC) model and the AF Ising model on triangular lattice. We estimate the exact critical magnetic fields for both models at zero temperature using the Wang-Landau sampling method. We also show the phase diagrams and the critical lines for the models using the joint density functions. We find that the shapes of critical lines for the models are identical, but the phase transitions across the critical lines are different.

1. Introduction

Monte Carlo simulations currently play a major role in statistical physics to study phase transitions and critical properties. They are well-known in the case of anti-ferromagnetic (AF) Ising on square lattice. However, the studies of frustrated systems such as triangular lattice [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18] is also highlighted by the difficult tasks to understand the various phenomena. It has been reported that AF Ising models have three types of conjectured patterns of critical lines [19]. The Blume-Capel (BC) model [20, 21, 22, 23, 24, 25] has been studied to understand systems such as metamagents, ternary alloys, and multicompent fluids. This spin-1 Ising model shows first-order transitions and second-order transition. In this paper, we study the critical lines and properties of the AF BC model as well as those of the AF Ising model on triangular lattice using the Wang-Landau sampling method [26, 27, 28, 29] and microcanonical analysis [1].

2. Model and Simulation

The Hamiltonian of the AF Ising model defined on $L \times L$ square lattice in two dimensions is given by

$$\mathcal{H} = -JE - hM, \tag{1}$$

where $E = \sum_{\langle i,j \rangle} \sigma_i \sigma_j$, $M = \sum_i \sigma_i$, $\sigma_i = \pm 1$, J is a negative coupling constant, and h is an external magnetic field. The Hamiltonian of the AF BC model is as follows:

$$\mathcal{H} = -JE - hM + DM^2, \tag{2}$$

where D is the crystal field (also called the single-spin anisotropy parameter or the spin impurity chemical potential), $M^2 = \sum_i {\sigma_i}^2$, and $\sigma_i = -1, 0$, or 1. Here, a negative coupling constant ($J < 0$) defines the AF BC model. The physical origin of the crystal field D arises from the non-central potentials for the metal atoms coordinated with various ligands in the crystal.

Using the WL algorithm, the $3d$ random walks are performed in the joint space [30, 31] $A = (E, M)$ for AF Ising model and $A = \left(E, M, M^2\right)$ for AF BC model by randomly changing the states of spins A, where the order parameter M is $\sum_i S_i$ and the square of order parameter M^2 is $\sum_i {S_i}^2$, but the state A associated with each spin configuration is only accepted with a probability proportional to the reciprocal of the joint density of states $g\,(A)$ [30, 31, 32, 33].

Therefore, the transition probability from state A to A' is

$$p\left(A \to A'\right) = min\left(\frac{g(A)}{g(A')}, 1\right), \tag{3}$$

which indicates that if $g\,(A') \le g\,(A)$, a state with spin configuration A' is always accepted, and that if $g\,(A') > g\,(A)$, it is accepted with the probability $g\,(A)\,/g\,(A')$.

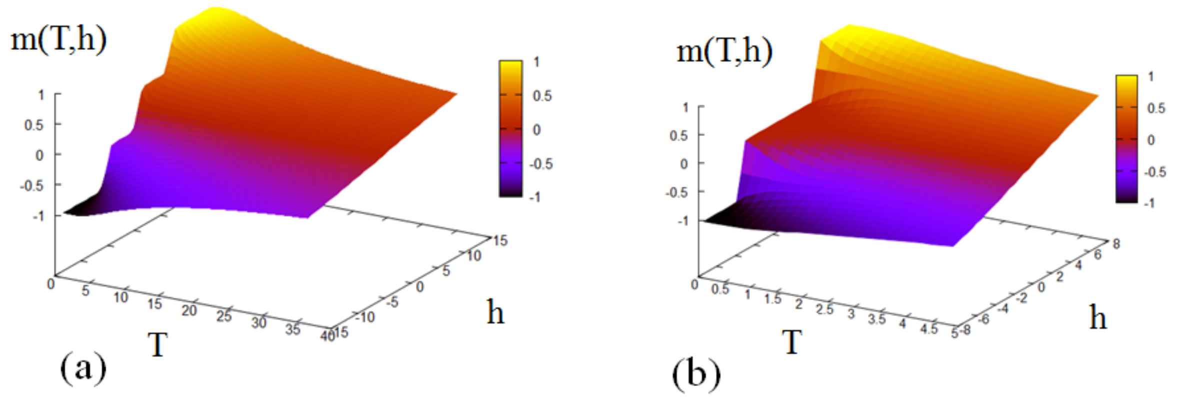

Figure 1. Magnetization m of (a) AF Ising model with $L = 12$ and (b) AF BC model with $L = 6$ as a function of energy, temperature, and h field on triangular lattice.

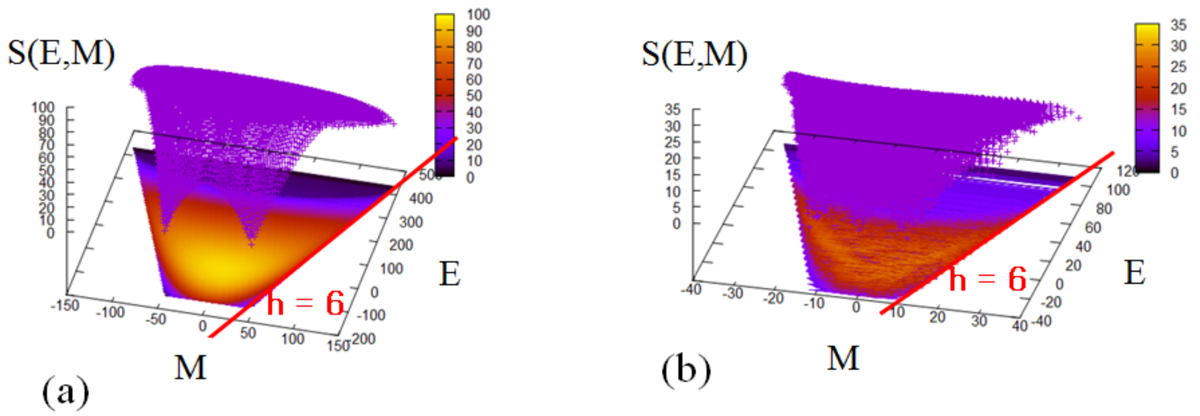

Figure 2. Microcanonical entropy of (a) AF Ising model with $L = 12$ and (b) AF BC model with $L = 6$ as a funcion of energy and magnetization on triangular lattice.

3. Results and Discussion

The canonical distributions of magnetization m for AF Ising model with linear dimension $L = 12$ and AF BC model with $L = 6$ on on triangular lattice are shown in figure 1. The line of m

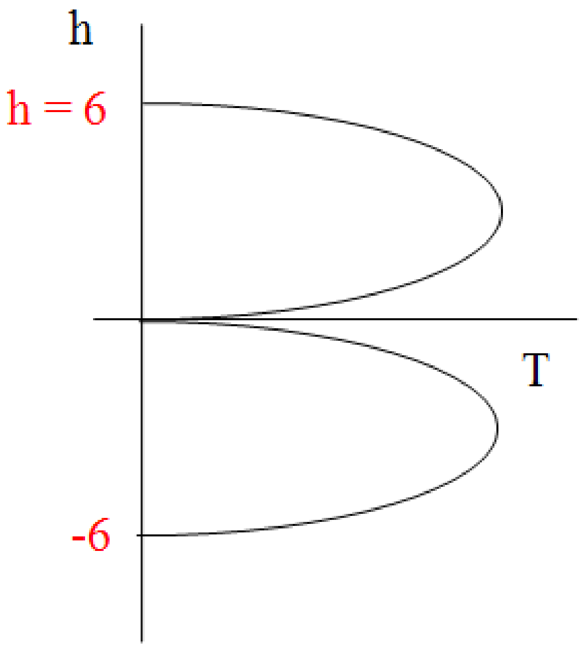

Figure 3. Schematic plot of three types of critical lines of AF Ising model with $L = 12$ and AF BC model with $L = 6$ on triangular lattice.

as a function of h in the vicinity of $T \sim 0$ shows discontinuity for AF BC model, but it does not show for AF Ising. Figure 2 shows microcanonical entropy $S(E, M)$ of (a) AF Ising model with $L = 12$ and (b) AF BC model with $L = 6$ as a funcion of energy and magnetization on triangular lattice. In Figure 2, the contour plot of ME diagram has four vertices. The top-left vertice corresponds to the state of all spins up. The locations of top-right vertices are as follows: $E = 432$ and $M = 144$ for AF Ising model, and $E = 102$ and $M = 35$ for AF BC model. In the contour plot of ME diagram in Figure 2, bottom line corresponds to the frustrated AF ground state without h. The locations of bottom-right vertices are $E = -144$ and $M = 48$ for AF Ising model, and $E = -36$ and $M = 12$ for AF BC model.

We can observe that at zero temperature the term with the minimum E_t is dominant, where $E_t = E - hM$ is the total energy. The total energy E_t can be interpreted as the intersection on the E axis of the linear line $E = hM + E_t$ in the ME diagram. Note that the slope of the line connecting the top right vertex and the bottom right vertex is six which is the critical magnetic field h_c, where $h_c = 6$ for AF Ising and AF BC models on triangular lattice.

Figure 3 shows the estimated critical lines of the AF Ising and AF BC models on triangular lattice. Although the patterns of critical lines for both models are the same, the transitions in the vicinity of $T \sim 0$ are different from each other. As shown in Figure 3, the critical line of AF BC model at $T \sim 0$ and $h = 6$ indicates the first order phase transition, whereas that of AF Ising at $T \sim 0$ and $h = 6$ indicates the second order phase transition.

4. Conclusions

In this paper, we study the AF BC and AF Ising model on triangular lattices using Wang-Landau sampling method and micro-canonical anaysis. We find critical lines of both models and find the critical magnetic field $h_c = 6$ at zero temperature. We also find that the critical line of AF BC model at $T \sim 0$ indicates the first order phase transition and that of AF Ising indicates the second order phase transition. Thus, our future intention is to extend the present investigations to the critical properties and phenomena of AF BC model on triangular lattice with non-zero D and non-zero h field.

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