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To cite this article: Chi-Ok Hwang *et al* 2016 *J. Phys.: Conf. Ser.* **750** 012016

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Study of the Antiferromagnetic Blume-Capel Model on kagomé Lattice

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Abstract.

We study the anti-ferromagnetic (AF) Ising model and the AF Blume-Capel (BC) model on the kagomé lattice. Using the Wang-Landau sampling method, we estimate the joint density functions for both models on the lattice, and we obtain the exact critical magnetic fields at zero temperature by using the micro-canonical analysis. We also show the patterns of critical lines for the models from micro-canonical analysis.

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 [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18] and kagomé lattices [19, 20] are also highlighted by the difficult task to understand the various phenomena. It has been reported that AF Ising models have three types of conjectured patterns of critical lines [21]. The Blume-Capel (BC) model [22, 23, 24, 25, 26, 27] has been studied to understand systems such as metamagnets, ternary alloys, and multicomponent 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 the kagomé lattice using the Wang-Landau sampling method [28, 29, 30, 31] 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

$$\mathcal{H} = -JE - hM, \quad (1)$$

where $E = \sum_{\langle i,j \rangle} \sigma_i \sigma_j$ and $M = \sum_i \sigma_i$, and $\sigma_i = \pm 1$. $J < 0$, and h is an external magnetic field. The Hamiltonian of the AF BC model is as follows:

$$\mathcal{H} = -JE - hM + DM^2, \quad (2)$$

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 [32, 33] $A = (E, M)$ for the AF Ising model and $A = (E, M, M^2)$ for the 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 $g(A)$ [32, 33, 34, 35].

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

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

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

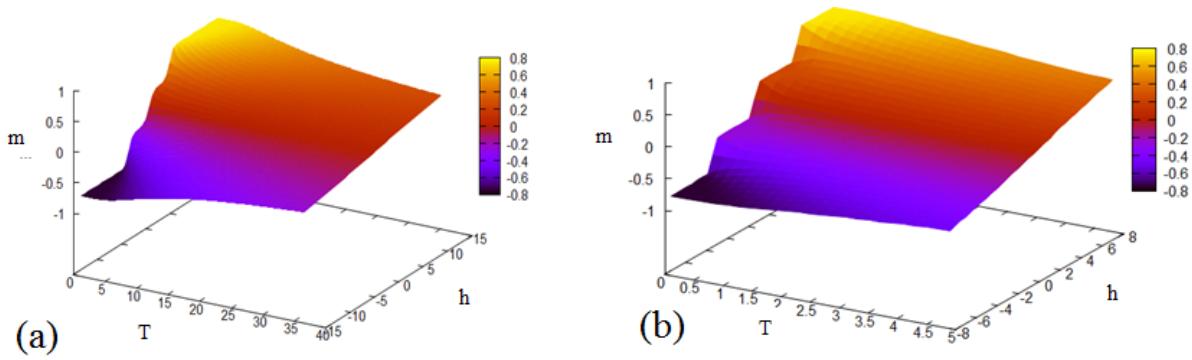


Figure 1. Magnetization m of (a) AF Ising model with $L = 12$ and (b) AF BC model with $L = 6$ as a function of energy, temperature, and h field on kagomé lattice.

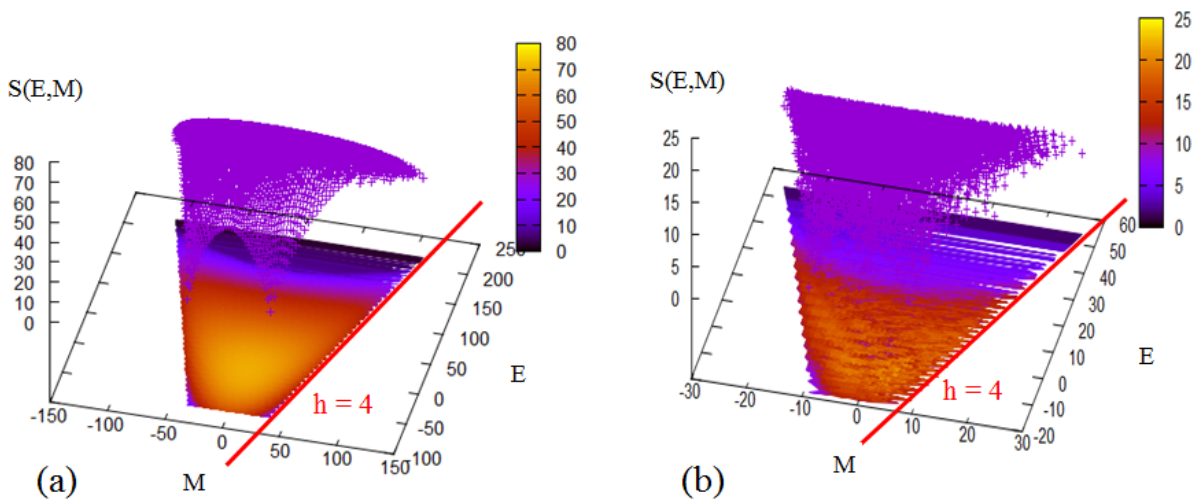


Figure 2. Microcanonical entropy of (a) AF Ising model with $L = 12$ and (b) AF BC model with $L = 6$ as a function of energy and magnetization on kagomé lattice.

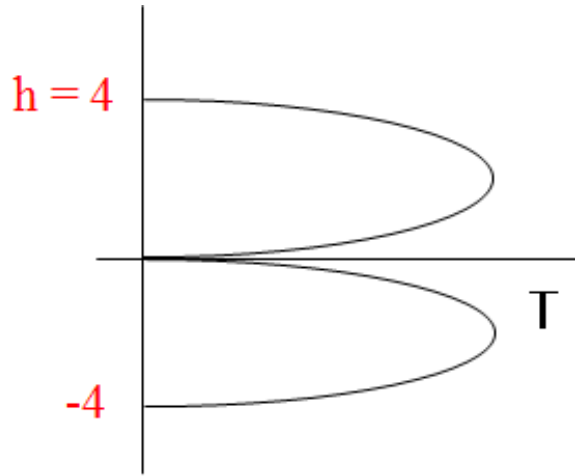


Figure 3. Schematic plot of three types of critical lines of a) AF Ising model with $L = 12$ and (b) AF BC model with $L = 6$ on kagomé lattice.

3. Results and Discussion

The canonical distributions of magnetization $m = M/L^2$ for AF Ising model with linear dimension $L = 12$ and AF BC model with $L = 6$ on kagomé lattice are shown in figure 1. The line of m 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 function of energy and magnetization on kagomé lattice. In Figure 2, the contour plot of the ME diagram has four vertices. The top-left vertex corresponds to the state of all spins up. The locations of top-right vertices are as follows: $E = 216$ and $M = 108$ for AF Ising model, and $E = 54$ and $M = 27$ for AF BC model. In the contour plot of the ME diagram in Figure 2, the bottom line corresponds to the frustrated AF ground state without h . The locations of bottom-right vertices are $E = -72$ and $M = 36$ for AF Ising model, and $E = -18$ and $M = 9$ 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 $h_c = 4$ for AF Ising and AF BC models on kagomé lattice.

Figure 3 shows the estimated critical lines of the AF Ising and AF BC models on kagomé 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 $h = 4$ indicates the first order phase transition, whereas that of AF Ising at $T \sim 0$ and $h = 4$ indicates the second order phase transition.

4. Conclusions

In this preliminary study by using the small kagomé lattices, we study the AF BC and the AF Ising model on kagomé lattices using the Wang-Landau sampling method and micro-canonical analysis. We find critical lines of both models and find the critical magnetic field $h_c = 4$ 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 the AF BC model on the kagomé lattice with nonzero D and non-zero h field.

Acknowledgment

This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education Science and Technology (NRF-2013R1A1A2065043 for W.Kwak) and was also supported by the Research support projects for distinguished professors through a grant provided by GIST in 2016 (Grant No. GK03872 for C.-O.Hwang). In addition, this research has been performed as a collaborative research project of project No (Supercomputing infrastructure service and application for C.-O.Hwang) and supported by the KOREA INSTITUTE of SCIENCE and TECHNOLOGY INFORMATION (KISTI).

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