Phase transitions of 2D triangular antiferromagnetic Ising model in a uniform magnetic field near $h=0$ and $T=0$

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Abstract. Using a microcanonical magnetization–energy (ME) diagram, this paper describes all the possible phase transitions of a 2D triangular antiferromagnetic (TAFM) Ising model in a uniform external magnetic field. In particular, we investigate the detailed phase boundary shape of the TAFM near $h=0$ and $T=0$ using staggered susceptibility.

1. Introduction

The 2D isotropic triangular antiferromagnetic (TAFM) model with no magnetic field has been solved fully. It has highly degenerate ground states, and there is no disorder–order phase transition [1]. However, an external magnetic field induces a long-range order with one-third magnetization because of the frustration. In the long-range order, there are two sublattices aligned to the field (called the $\alpha$ sublattices) and one sublattice (called the $\beta$ sublattice) anti-aligned to the field [2] (see Figure 1). Here, we consider the triangular-lattice Ising antiferromagnet in a uniform external magnetic field, with the Hamiltonian $H = -J \sum_{i,j>\langle} \sigma_i \sigma_j - h \sum_{i=1}^{N} \sigma_i \ (J < 0). < i, j >$ denotes distinct pairs of nearest-neighbor sites.

![Figure 1. Long-range order example.](image.png)
In [3-6], it was found that there is a field-induced Kosterlitz–Thouless (KT) transition to a long-range-ordered state at a field $H_c = 0.266 \pm 0.010$ at the limit of $h \to 0$ and $T \to 0$, keeping $H = h/T$, a constant. Even though this 2D frustrated system is a classical problem, and many advanced frustrated systems have been well investigated [7], it still seems that we do not understand the classical problem completely yet. Besides the KT transition, there is another phase transition belonging to the three-state Potts universality class [8]. However, around the point $h = 0$ and $T = 0$, we do not know where the three-state Potts transition starts, because the crossover effect degrades the convergence. In addition, we do not know why we have two different transition types on the TAFM, because from the microcanonical ME diagram, we can expect only one type. In addition, if we use another order parameter, we do not know what will happen (see Figure 4).

Besides the usual total magnetization order parameter $\sum_i \sigma_i$, we can use another order parameter, so-called staggered magnetization $\sum_{i \in \beta} \sigma_i - \sum_{j \in \alpha} \sigma_j$, so that the order parameter ranges from -1 to 1. If we use this order parameter, in any given plaquette, two sublattices will have the same average value of spin, and the order parameter will be a 2D one made up of appropriate combinations of the sublattice magnetizations. Hence, the ground state in a magnetic field is degenerate. A long time ago in a previous research study, a phase diagram was obtained using staggered magnetization [2].

In our previous research [9], we obtained the density of states (DOS) $g(M,E)$ as a function of the energy (E) and magnetization (M) of the TAFM using the exact enumeration method for small systems and the Wang–Landau method for larger systems (see Figure 2). From the top view of the DOS, we could obtain the magnetization–energy (ME) diagram (see Figure 3).

In this paper, on the microcanonical ME diagram, we describe all the possible phase transitions of the 2D TAFM Ising model in a uniform magnetic field and investigate the detailed phase boundary shape of the TAFM near $h=0$ and $T=0$.

![Figure 2. Example of density of states (DOS) with size $L = 10$ [5].](image1)

![Figure 3. Magnetization–Energy (ME) diagram of TAFM with size 12x12 [5]. Solid colored lines are shown for the ground states with external magnetic fields.](image2)

2. Phase transitions of ground states

To understand the phase transitions of ground states, it is very useful to use the ME diagram obtained by Wang–Landau sampling. From the ME diagram, we can understand all the ground states in external magnetic fields. From the Hamiltonian $E_f = E - hM$, we can notice that the external magnetic field is the slope on the ME diagram. On the diagram, we can clearly see that the external magnetic field $h = 6$ is the critical magnetic field, where the ground state can be mapped onto the Baxter’s hard-
hexagon lattice gas [10], and there are four critical ground–state points: $E_{\text{min}} = L^2$ and $M = 0$ when $h = 0$, $E_{\text{min}} = L^2$ and $M = L^2/3$ when $0 < h < 6$ (long-range order), $E = L^2$ and $M = 2L^2/3$ when $h = 6$, and $E = 3L^2$ and $M = L^2$ when $h > 6$ (here, $L$ is the lattice size). According to the given field change, such as from $h = 0$ to any magnetic field in $0 < h < 6$, we can see a phase transition from one ground state to another.

3. Phase boundary shape of TAFM near $h=0$ and $T=0$

The field-induced KT transition at the limit of $h \rightarrow 0$ and $T \rightarrow 0$ keeping $H = h/T$ a constant can be interpreted as the tangent slope of the phase boundary at $h=0$ and $T=0$. The tangent slope at the point is not zero, and it means that with a nonzero small external magnetic field at the ground state, the system does not go to the long-range order immediately but the magnetic field strength is marginal (see Figure 5). In our previous research [11] we confirmed the critical value $H_c$ using normal magnetization susceptibility with Wang–Landau sampling (see Figure 6).

Figures 4 and 5 are different, because they use different order parameters. The two magnetic lines in Figure 5 show that with a nonzero small external magnetic field at the ground state, the system does not go to the long-range order immediately [5].

For staggered susceptibility, we can use the variance of $\sum_{i \in B} \sigma_i - \sum_{j \in \alpha} \sigma_j$ as an ordering parameter. In this case, we need the more expanded DOS, $g(M_1, M_2, E)$, where $M_1 = \sum_{i \in B} \sigma_i$ and $M_2 = \sum_{j \in \alpha} \sigma_j$. We had difficulty using Wang–Landau sampling because of the high dimension of the DOS and thus used Metropolis sampling to obtain Figures 7 and 8. We started the TAFM from the long-range order state and slowly increased the temperature. After reaching the equilibrium, we collected the data. In Figure 7, we have two peaks corresponding to the KT phase transition (right peak) and another boundary, we suspect, related to Burley’s Kikuchi approximation (left peak) [12]. It seems that the two peaks diverge with respect to the linear system size. In future research, to take full advantage of Metropolis sampling, we will perform simulations with much bigger sizes up to the linear system sizes, such as 513 and 1026.
Figure 6. Normal magnetization susceptibility with Wang–Landau sampling [12].

Figure 7. Staggered susceptibility with $L = 30$ and $h = 0.2$ using Metropolis algorithm.

Figure 8. Staggered susceptibility maxima vs. lattice sizes.
4. Conclusion and further research

In this research, we used the ME diagram to understand all the possible phase transitions at ground states, and we investigated the detailed phase boundary shape of the TAFM near $h=0$ and $T>0$ using staggered susceptibility and confirmed the KT transition at the limit of $h \to 0$ and $T \to 0$. However, in our preliminary research results, we could also see another phase boundary line.

In our future research, we will investigate the phase boundary with bigger linear system sizes. In addition, we will investigate the phase transitions via microcanonical entropy inflection points. We hope to determine where the two phase transitions cross over on the phase boundary.

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