Phase transitions in the frustrated antiferromagnetic XY model on the triangular lattice

M Klawtanong\(^1\) and C Srinitiwarawong\(^2\)
\(^1\)Department of Physics, Faculty of Science, Ramkhamhaeng University, Ramkhamhaeng Road, Bang Kapi, Bangkok 10240, Thailand
\(^2\)Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand
E-mail: manit.k@ru.ac.th

Abstract. Phase transitions and thermodynamics properties of the frustrated antiferromagnetic XY (FAXY) model have been investigated near the two transition temperatures. We found that the Kosterlitz-Thouless (KT) transition corresponding to the rotational $U(1)$ symmetry breaking and the Ising-like (I) transition corresponding to the reflection $Z_2$ symmetry breaking occur at two-separate transition temperatures, $T_{KT} < T_I$. These temperatures lie close to each other, however in our results the separation is obvious. Our results show the order parameters as a function of temperature and we also estimate the critical exponents, $\beta$, $\alpha$, $\gamma$, $\eta$ and $\nu$. The critical exponent $\nu$ indicates that the Ising-like transition is inconsistent with the Ising universality class.

1. Introduction
Frustrated spin systems have been one of the topics studied in the last two decades. They play an important role in a study of the critical phenomena in a wide range of physical systems. A few interested models that have been investigated via the simulation methods and also theoretical studies are the fully frustrated XY (FFXY) model [1–4], the frustrated antiferromagnetic XY (FAXY) model [3, 5] and the frustrated antiferromagnetic six-state clock model [6, 7]. These models describe the orientational ordering transition of CF$_3$Br molecules on graphite [6]. The frustrated XY models have a rotational $U(1)$ symmetry and an additional reflection $Z_2$ symmetry that can be broken at the Kosterlitz-Thouless (KT) and an Ising-like (I) transition temperatures, $T_{KT}$ and $T_I$, respectively. Since the non-frustrated XY model has been quite well known, therefore the additional $Z_2$ symmetry breaking transition has been the subject of interest in these models.

Interestingly, it has not been exactly known whether this transition belongs to the Ising universality class or not [1–3, 5–7]. The $T_I$ occurs closely to the $T_{KT}$ [2–7] which are possibly merged into a single transition with a new universality class [1–3, 7]. Moreover the specific heat was found to exhibit the power law behavior rather than the logarithmic behavior [1, 3] suggesting a non-Ising universality class. In this study, we investigate the critical behavior of the FAXY on the triangular lattice using the Monte Carlo simulation methods and the Metropolis algorithm [8]. Our aims are to identify the transition temperatures, to estimate the critical exponents and to classify the universality class of the Ising-like transition.
2. Model and method

Figure 1(a) shows FAXY model on a triangular lattice. The Hamiltonian of the system is given by

\[ H = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j), \]  

(1)

where \( J < 0 \) is the exchange energy, the sign \( \langle i,j \rangle \) denotes a sum over nearest neighbor spins, \( \mathbf{S}_i \) is a classical vector spin with \( |\mathbf{S}_i| = 1 \) and \( \theta_i \) is the spin angle respected to an arbitrary direction. We use the periodic boundary conditions with linear system sizes \( N = L \times L \). To create a stochastic process, the Monte Carlo (MC) method and Metropolis algorithm are needed [8].

The system is initially set in high (low) temperature states after that we decrease (increase) temperature \( T \equiv k_B T/|J| \) to final temperature. The system will be discarded at earlier time until it reaches new equilibrium states. We measure variables every 2, 5 and 10 MC time steps and all variables will be averaged over at least 100,000 microstates.

The order parameters for \( U(1) \) and \( Z_2 \) symmetry breaking transitions are sublattice magnetization \( m \) and staggered chirality \( h \)

\[ m = \frac{1}{3N} \left\langle \left| \sum_A \mathbf{S}_i \right| \right\rangle, \]

\[ h = \frac{1}{2N} \left\langle \sum_A (h_{\triangle_i} - h_{\nabla_i}) \right\rangle. \]

(2)

(3)

The sums run only over sites \( i \) in sublattice \( A \) and \( \langle \ldots \rangle \) denotes an average over all states. The chiralities \( h_{\triangle_i,\nabla_i} \) for up- and down-triangles \( i \) in figure 1(a) are given by [5,6]

\[ h_{\triangle_i,\nabla_i} = \frac{2}{3\sqrt{3}} [\sin(\theta_m - \theta_l) + \sin(\theta_n - \theta_m) + \sin(\theta_l - \theta_n)]. \]

(4)

The Binder cumulants [8] for the magnetization and chirality denoted by \( B_m \) and \( B_h \) are used to determine \( T_{KT} \) and \( T_I \), respectively. Specific heat \( C_V \) and magnetic susceptibility \( \chi_m \) can be obtained from the energy and sublattice magnetization fluctuations [8]. Finally, the chirality correlation \( C_h(r) \) and its correlation length \( \xi_h \) are determined using

\[ C_h(r) = \frac{3}{N} \left\langle \sum_A h_{\triangle_i} h_{\triangle_{i+r}} \right\rangle, \]

\[ \xi_h = \sqrt{\sum_r r^2 C_h(r)/\sum_r C_h(r)}, \]

(5)

(6)

where \( i + r \) denotes a site displaced by distance \( r \) in the vertical direction from site \( i \).

3. Results

3.1. Critical temperatures

Figure 1(b) shows \( B_m \) versus temperature \( T \) for different system sizes \( L \times L \). At a critical point, where \( B_m \) becomes independent of system sizes, \( T_{KT} \) is estimated to be 0.509(8) and is marked by the solid line. In figure 1(c), \( T_I \) can be determined in the same manner, which is \( T_I = 0.513(0) \) (dashed line). From the results, it is clearly shown that the system has two separate transitions with \( T_{KT} < T_I \). The transitions at two different temperatures have been observed in the frustrated XY models [2,3,5–7].
3.2. Order parameters and exponents

Order parameter $m$ for sublattice magnetization increases as decreasing $T$ and it approaches a saturated value as $T \to 0$. For a finite system size, $m$ depends on $L$ as $m \sim L^{-x}$ with finite size scaling $x = 1/8$. Figure 2(a) shows $m$ as a function of $L$. The high and low temperatures are separated by the dashed line at $T_{KT}$ with $x = 0.16$. The value is higher than 1/8 but is in good agreement with those results [6]. Order parameter $h$ also exhibits a scaling behavior $h \sim (-t)^\beta$ near a critical point, where $t = (T - T_I)/T_I$ is a reduced temperature and $\beta$ is a critical exponent. This behavior is only true at low temperature. The dashed line in figure 2(b) shows a power law of $h$ for $L = 120$ with $\beta = 0.125$. This value is in good agreement with the

![Figure 1](image1.png)

**Figure 1.** (a) A $6 \times 6$ triangular lattice with $A$, $B$ and $C$ sublattices. The ± signs denote the chirality at each triangle and the shaded triangles refer to up- and down-triangles $i$ denoted by $\Delta_i$ and $\nabla_i$, respectively. Binder cumulants: (b) $B_m$ and (c) $B_h$ versus $T$ for various lattice sizes. The solid and dashed lines mark $T_{KT} = 0.509(8)$ and $T_I = 0.513(0)$, respectively.

![Figure 2](image2.png)

**Figure 2.** (a) $m$ as a function of $L$ with a power law decay (dashed line) at $T = T_{KT}$ (filled triangle). (b)-(d) $h$, $C_V$, and $\chi_m$ as a function of $t$ for various $L$. Dashed lines indicate power behaviors with critical exponents $\beta$, $\alpha$, and $\gamma$, respectively. (e) Correlation function $C_h$ as a function of $r$ at $T_I$ with exponent $\eta$ (dashed line). The inset shows $\eta$ dependent on $1/L$ (solid line). (f) $\xi_h$ as a function of $t$ with $\nu = 0.74$ (dashed line) and $\nu$ as a function $1/L$ (solid line in the inset).
Ising value of \( \beta = 1/8 \).

Fluctuations of the energy and sublattice magnetization near a critical point determine specific heat \( C_V \) and magnetic susceptibility \( \chi_m \) of the system. Figures 2(c)-(d) show \( C_V \) and \( \chi_m \) as a function of reduced temperature \( t \). The specific heat also has scaling behavior, however, there has been no consensus on its behavior, power law behavior [1,3] as \( C_V \sim t^{-\alpha} \) or logarithmic behavior [6] as \( C_V \sim \log|t| \) with critical exponent \( \alpha = 0 \). To observe this behavior, \( C_V \) is plotted versus \( t \) in the log-log scale as shown in figure 2(c). It seems that \( C_V \) prefers a power law rather than a logarithmic law both above and below critical temperature. However, at \( t \to 0 \), the behavior does not occur evidently because of \( C_V \) dependent on \( L \) near the critical point. We estimate that \( \alpha = 0.45 \) for \( L = 120 \) at intermediate \( t \) (dashed line). Next, the critical behavior of \( \chi_m \) can be written as \( \chi_m \sim t^{-\gamma} \) with critical exponent \( \gamma \). We estimate \( \gamma \) to be \( \gamma = 1.05 \) for \( t < 0.1 \) and \( \gamma = 1.23 \) for \( t > 0.1 \) marked by the dashed lines in figure 2(d).

The behavior of correlation function \( C_h \) follows an exponential decay as \( C_h \sim r^{-\eta} \) at \( T_I \) with critical exponent \( \eta \). We estimate that \( \eta = 0.19 \) for \( L = 120 \) in figure 2(e). The value of \( \eta \) depends on system size \( L \). Using a linear best fit, \( \eta \) is approximated to be \( \eta \approx 0.22 \) in the limit of \( 1/L \to 0 \) indicated by the solid line in the inset. Finally, the correlation length of chirality given by equation (6) increases with decreasing \( t \) as \( \xi_h \sim |t|^{-\nu} \). Critical exponent \( \nu \) is estimated to be \( \nu = 0.74 \) marked by the dashed line for \( L = 120 \) in figure 2(f). The value of \( \nu \) also depends on system size \( L \). To obtain \( \nu \) in the limit of \( L \to \infty \), we plot \( \nu \) versus \( 1/L \) in the inset and estimate the value of \( \nu \) using a linear best fit to be \( \nu \approx 0.83 \) as \( 1/L \to 0 \) (solid line).

In summary, for the Kosterlitz-Thouless transition, we estimate that \( x = 0.16 \) at \( T_{KT} \), \( \alpha = 0.45 \), and \( \gamma = 1.05(1.23) \) for \( t < 0.1(t > 0.1) \). The critical exponents of the Ising-like transition from our results compared to those results in the references are listed in Table 1.

**Table 1.** Critical exponents of the Ising-like transition.

| Exponent | This work | Ref. [1] | Ref. [2] | Ref. [3] |
|----------|-----------|----------|----------|----------|
| \( \beta \) | 0.125 | 0.12 | 0.106 | 0.11 |
| \( \eta \) | 0.22 | - | 0.250 | - |
| \( \nu \) | 0.83 | 0.83 | 0.84 | 0.83 |

4. Conclusion

In conclusion, we show clearly that the system has two separate transitions with \( T_{KT} < T_I \). These temperatures lie very close to each other, about 0.6% compared to lower temperature. We estimate various exponent values for both transitions. For the Ising-like transition, the values are shown in Table 1. It seems that the Ising-like transition with \( \nu = 0.83 \) is inconsistent with the Ising universality class.

**References**

[1] Lee J, Kosterlitz J M and Granato E 1991 Phys. Rev. B 43 11531
[2] Ozeki Y and Ito N 2003 Phys. Rev. B 68 054414
[3] Lee S and Lee K-C 1998 Phys. Rev. B 57 8472
[4] Lima A B, MóI L A S and Costa B V 2019 J. Stat. Phys. 175 960
[5] Lv J-P, Garoni T M and Deng Y 2013 Phys. Rev. B 87 024108
[6] Noh J D, Rieger H, Enderle M and Knorr K 2002 Phys. Rev. E 66 026111
[7] Surungan T, Okabe Y and Tomita Y 2004 J. Phys. A 37 4219
[8] Landau D P and Binder K 2000 *A Guide to Monte Carlo Simulations in Statistical Physics* (Cambridge: Cambridge University Press)