Journal of Magnetism and Magnetic Materials 340 (2013) 127–130

Contents lists available at SciVerse ScienceDirect

Journal of Magnetism and Magnetic Materials

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

Phase diagram of ferromagnetic *XY* model with nematic coupling on a triangular lattice

K. Qi [a,b], M.H. Qin [a,*], X.T. Jia [c], J.-M. Liu [b,**]

[a] Laboratory for Advanced Materials, South China Normal University, Guangzhou 510006, China
[b] Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, China
[c] School of Physics and Chemistry, Henan Polytechnic University, Jiaozuo 454000, China

ARTICLE INFO

Article history:
Received 11 December 2012
Available online 9 April 2013

Keywords:
XY model
Kosterlitz–Thouless transition
Monte Carlo simulation

ABSTRACT

The phase diagram of a ferromagnetic *XY* model with a nematic coupling (coupling strength x) on a triangular lattice is studied by means of Monte Carlo simulation. The algebraic-magnetic order associated with Kosterlitz–Thouless (KT) transition is observed over the whole x range. In the large x region, the phase transition from the algebraic-magnetic order to the algebraic-nematic order occurs at T_I. In addition, this phase transition can be scaled with the two-dimensional Ising critical exponents, demonstrating that the present system belongs to the universality class of Ising transition at T_I.

1. Introduction

The two dimensional (2D) *XY* model has been well investigated for several decades due to its application in magnetic systems with planar anisotropy, quantum liquids and superconductors. As early as in 1966, it was proved that the 2D *XY* model cannot sustain long-range order even with trivial thermal fluctuations [1]. Alternatively, the so-called algebraic-magnetic (aM) order with Kosterlitz–Thouless (KT) transition may ensue [2,3]. After that, lots of work about the *XY* model have been reported [4–18].

On the other hand, nontrivial orders such as chiral order and nematic order in magnets, are drawing more and more attentions due to their relevancy with real magnetic materials as well as the contribution to the development of statistical mechanics. For example, a phase with coexisting nematic and vector spin chirality orders has been observed in the antiferromagnetic *XY* model with a nematic (biquadratic) coupling on the triangular lattice [7]. Later on, the same phase is also reported in our earlier work where a frustrated *XY* model on the square lattice has been studied with the Monte Carlo method [8]. In fact, the ferromagnetic *XY* model with a nematic coupling on square lattice has been studied as early as in 1989 [5]. The variations of temperature and the nematic coupling strength lead to three phases: a high-temperature disordered phase and two low temperature phases, namely, aM phase and algebraic-nematic (aN) phase. At non-zero temperatures, spin waves destroy the long-range order of the ground state, leaving power-law decay of the spin correlations. The high-temperature phase is entered respectively via the transition associated with an integer vortex pair excitation in the aM phase and an half-integer vortex pairs one in the aN phase [9]. At the same time, it is stated that the phase transition from disordered phase to aN phase is driven by the domain wall in which the free energy is expected to decrease with increasing temperature.

In fact, the consideration of the nematic coupling terms is mostly due to the fact that they can be large for magnetic ions with large spin [19]. For example, it is identified that the nematic coupling and the ferromagnetic coupling between the nearest neighbors may play an important role in triangular lattice system $NiGa_2S_4$, as revealed most recently [20]. In this work, a ferromagnetic *XY* model with a nematic coupling (coupling strength x) on a triangular lattice is studied by means of Monte Carlo simulation. Besides its contribution to the development of statistical mechanics, the study may be helpful to understand the experimental phenomena observed in $NiGa_2S_4$. As far as we know, few works on such a system have been reported. It will be demonstrated that a general KT transition from the algebraically correlated phase to the paramagnetic phase occurs when temperature raises up to a critical value. For the region in which the nematic coupling is dominated, a transition from the aM phase to the aN phase occurs at the critical temperature T_I which is much lower than T_{KT}. In addition, the transition at T_I has the same universality of scaling as the two-dimensional (2D) Ising transition, which is similar to earlier report [5].

For a classical *XY* spin model on a triangular lattice, we consider the following Hamiltonian which includes the nematic coupling interaction:

$$H = -J_1 \sum_{[i,j]} \cos(\theta_{ij}) - J_2 \sum_{[i,j]} \cos(2\theta_{ij}), \tag{1}$$

* Corresponding author. Tel.: +86 13632457166.
** Corresponding author.
E-mail addresses: qinmh@scnu.edu.cn (M.H. Qin), liujm@nju.edu.cn (J.-M. Liu).

0304-8853/$ - see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.jmmm.2013.03.036

where θ_{ij} is the angle difference θ_i–θ_j between the nearest neighbors [i,j]. $J_1=1-x$ is the strength of the ferromagnetic coupling, and $J_2=x$ is the nematic coupling strength. For definition of the energy parameters J_1 and J_2, the Boltzmann constant and the lattice constant are set to unity.

Unlike the model studied in Ref. [7], our model does not contain any chiral orders due to the lack of the frustration ingredient. In the large J_2/J_1 region where the nematic interaction is much stronger than the ferromagnetic one, the spins between the nearest neighbors prefer either parallel or antiparallel with each other at the equal probabilities at low temperature, forming the possible nematic order, same as the earlier report [5].

The Monte Carlo simulation is performed on a 2D $L\times L$ ($L=18$, 27, 36, 45, 54, and 72) triangular lattice with period boundary conditions using the standard Metropolis algorithm [21]. The initial spin configuration at high temperature (T) is totally disordered. Typically, the initial 3×10^5 Monte Carlo steps are discarded for the equilibrium consideration and another 2×10^5 Monte Carlo steps are retained for statistic averaging of the simulation.

The phase diagram in the x–T plane for the model stated in Eq. (1) is shown in Fig. 1. The two curves mark the boundaries between three different phases, which are the aM phase, aN phase and paramagnetic (PM) phase. An integer vortex-mediated KT transition marking the PM–aM boundary splits into a half-integer vortex-mediated KT transition which marks the PM–aN boundary, plus a transition which separates the aM order from the aN order. It is noticed that in the most cases the critical temperatures of the KT transition and Ising transition are relatively higher than the corresponding ones [5]. This phenomenon can be easily understood from the point that for the systems with the same ferromagnetic coupling, one with higher coordination number shows the higher critical temperature. It is noted that for triangular system one spin interacts with six nearest neighbors rather than four for square system. So, the algebraically correlated order in triangular system is so robust and its destruction needs relatively high temperature.

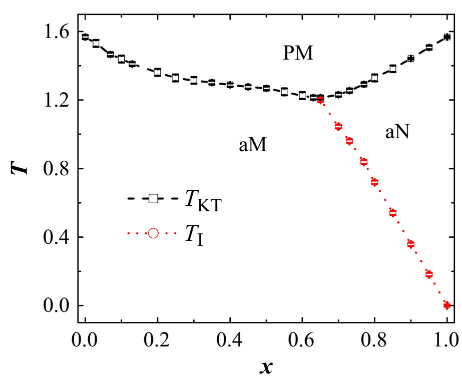

Fig. 1. Calculated phase diagram for the model in Eq. (1). The high-temperature paramagnetic phase is denoted by PM, the phases with algebraic correlations in magnetic and nematic order by aM and aN respectively. The statistical errors of all the symbols are given in the T direction.

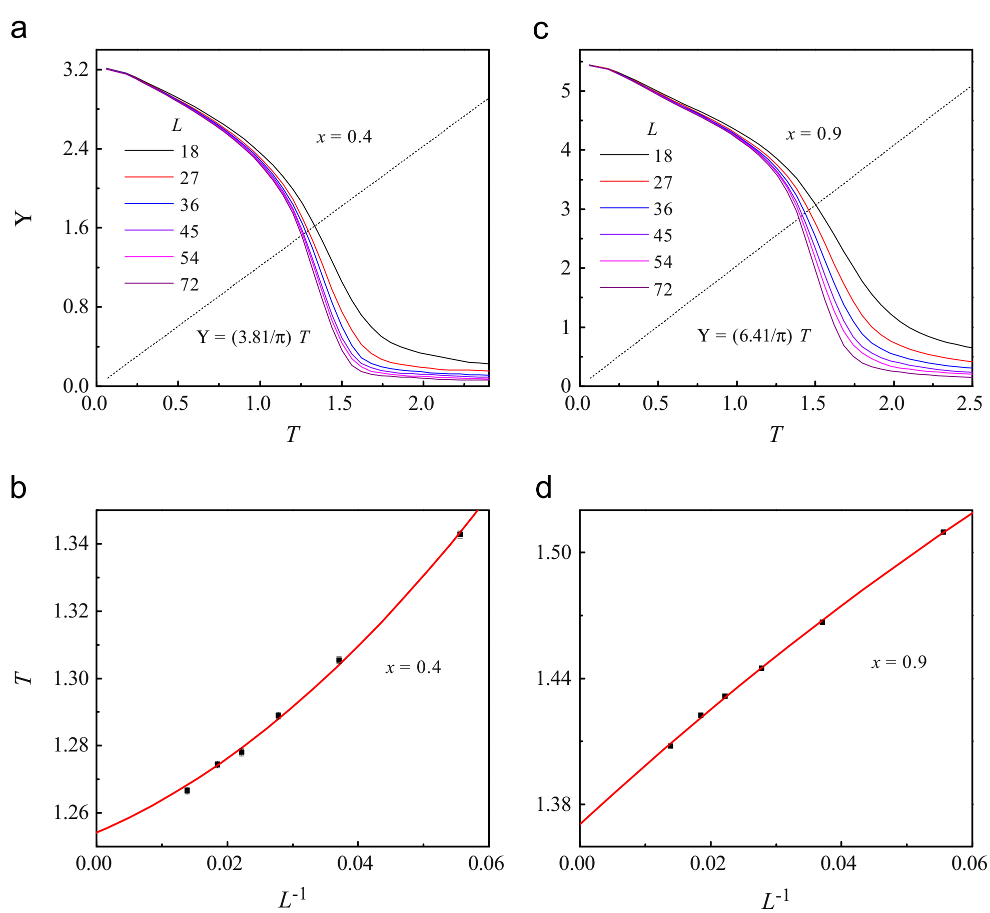

Fig. 2. Helicity modulus Υ according to Eq. (2) for various sizes L (a) at $x=0.4$ and (c) $x=0.9$. The straight line is $(2/\pi)(\sqrt{3}/2)(1+3x)T$. The crossing temperatures of this line and Υ for each L^{-1} are shown in (b) for $x=0.4$ and (d) $x=0.9$ with the extrapolation to $L^{-1}=0$.