A numerical study of the phase transition in a triangular-lattice model with three-spin interactions

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Abstract. We study a Berezinskii-Kosterlitz-Thouless-like phase transition in a triangular-lattice three-spin interaction model. The vector sine-Gordon field theory describes defects involved, and enables us to perform the renormalization-group analysis of the transition. Based on it, we discuss properties of the spin-spin correlation function, and also analyze the helicity modulus for the present model. To provide the data to support our analysis, we perform the Monte-Carlo simulations to calculate them. Further, we exhibit snapshots of some typical defect configurations, which are helpful to illustrate the defect-mediated phase transition.

Introduction.—In this report, we provide our recent investigation results on a three-spin interaction model introduced, long time ago, by Alcaraz et al [1, 2]. Suppose that \( \langle k, l, m \rangle \) denotes three sites at corners of each elementary plaquette of the triangular lattice \( \Lambda \) which consists of three sublattices \( \Lambda_a, \Lambda_b, \Lambda_c \), then the following Hamiltonian defines our model:

\[
\beta H = -\frac{J}{k_B T} \sum_{\langle k,l,m \rangle} \cos (\varphi_k + \varphi_l + \varphi_m), \quad \varphi_k \in [0, 2\pi).
\]  

The temperature \( T \) is measured in units of \( J/k_B \). The symmetry of the model is expressed by the global spin rotation, \( \varphi_k \rightarrow \varphi_k + \sum_{\rho=a,b,c} \sum_{l \in \Lambda_{\rho}} \psi_{\rho} \delta_{k,l} \) with the condition \( \psi_a + \psi_b + \psi_c = 0 \) (mod \( 2\pi \)). This \( U(1) \times U(1) \) symmetry with two independent phases (say \( \psi_{a,b} \)) is not broken, and gives a low-temperature critical phase, like the Berezinskii-Kosterlitz-Thouless (BKT) phase in the two-dimensional (2D) XY model [3]. But, it is of a criticality with the central charge \( c = 2 \). Furthermore, since topological defects involved are not described by the scalars (vortexes), but by vectors [2] like the Burgers vectors for the dislocations in the 2D melting [4], it is expected to exhibit a transition to the disordered phase in a different way to the \( c = 1 \) BKT case (see below). Thus, we shall here report our study on this novel phenomenon.

Theory.— According to reference [5], the following vector sine-Gordon Lagrangian density is relevant to an effective description:

\[
\mathcal{L} = \frac{K}{4\pi} \sum_{i=x,y} \| \partial_i \Phi(x) \|^2 + \frac{y_1}{2\pi a^2} \sum_{\| N \| = 1} : e^{i(N \cdot \Phi(x))} : .
\]  

\( \Phi(x) \) is a two component vector field attached at the position \( x \) in the basal 2D space, so the first term represents an interface model, where \( K \) roughly proportional to the inverse temperature, gives its stiffness (\( a \) is a short-distance cutoff). The above symmetry is realized as a periodicity
of the field, i.e., \( \Phi \equiv \Phi + 2\pi \mathbf{e}_\alpha (\alpha = 1, 2) \), where \( \{\mathbf{e}_{1,2}\} \) are normalized primitive vectors of the so-called repeat lattice \( \mathcal{R} \) [6] isomorphic to the triangular lattice [5]. Then, the interface can acquire the discontinuity of the amount \( 2\pi \mathbf{N} \) with \( \mathbf{N} \in \mathcal{R} \). The second term consists of vertex operators where \( ik \partial_i \Phi = \epsilon_{ij} \partial_j \Theta \), and creates shortest discontinuities among possible ones (i.e., the length \( ||\mathbf{N}|| = 1 \)). From the renormalization-group (RG) viewpoint, these topological defects controlled by an effective fugacity \( y_1 \) are enough to be kept in the theory because these are the most relevant ones. Since equation (2) takes the form of the perturbed conformal field theory, it is straightforward to perform its analysis using the operator-product-expansion coefficients: According to references [7, 8], RG equations for the change of the cutoff \( \alpha \rightarrow (1 + d\alpha) \) are given by \( dy_0(l)/dl = -3y_1(l)^2 \) and \( dy_1(l)/dl = -2y_0(l)y_1(l) - y_1(l)^2 \) where \( y_0 \equiv K/K^* - 1 \) with \( K^* \equiv 4 \). Like the BKT case, there is one separatrix \( y_1 = y_0 \) between the critical and the disordered phases, and thus effects of the defects cannot be renormalized to the stiffness constant on its upper side (see Fig. 1 in reference [7]).

To investigate the phase transition quantitatively, we shall focus on two physical quantities: (i) the spin-spin correlation function and (ii) the helicity modulus; both of them can be treated by the Monte-Carlo (MC) simulation method. For this issue, the bosonized expression of the spin degrees of freedom, \( S_k \equiv e^{iv_k} \), is important [5]: It takes a sublattice-dependent form, and is given by

\[
(S_{\alpha}, S_{\beta}, S_{\epsilon}) = (e^{i(e^1+e^2)\Phi}, \cdots, e^{-i(-e^1)\Phi}, \cdots, e^{-i(-e^2)\Phi}).
\] (3)

\( \{e^{1,2}\} \) are primitive vectors of the reciprocal lattice of \( \mathcal{R} \), \( \mathcal{R}^* \), and satisfy the duality relation \( \mathbf{e}_\alpha \cdot e^\beta = \delta^\beta_\alpha \). The correlation function between two spins on a same sublattice takes finite values, and it exhibits the power-law decay with the exponent \( \eta = 4/3K \) if the system is critical. However, it vanishes for two spins on different sublattices due to the vector charge neutrality condition [2, 5]. Also, owing to the expression, we can obtain a snapshot of the defect distribution \( \{N_k\} \) from a given phase variables \( \{\varphi_k\} \): Since \( \varphi_k \) in \( \Lambda_\alpha \) represents \( (e^1 + e^2) \cdot \Phi \), a nonzero vorticity around a certain elementary triangle of \( \Lambda_\alpha \) shows an existence of the defect within it [i.e., \( (e^1 + e^2) \cdot \mathbf{N} \neq 0 \)]. We shall denote the vorticity as \( v^1 \) \( (v^2) \) when the center site belongs to \( \Lambda_c \) \( (\Lambda_h) \). In the same way, we calculate the vorticity from \( \varphi_k \) in \( \Lambda_h \) \( (\Lambda_c) \), and denote it as \( v^1 \) \( (v^2) \) \( (v^3) \) \( (v^4) \) when the center belongs to \( \Lambda_\alpha \) \( (\Lambda_h) \) \( (\Lambda_c) \). Then, including zero, each site has two integers \( v^1 \) and \( v^2 \) (the sublattice index is dropped); using them we can put the defect vector on each site according to a sublattice dependent expression: \( \mathbf{N} = n^a_\mathbf{e}_a \) with

\[
(n^{1}_{\alpha}, n^{2}_{\alpha}) = (-v^1, -v^2), \ (n^{1}_{\beta}, n^{2}_{\beta}) = (v^1 + v^2, -v^1), \ \text{and} \ (n^{1}_{\epsilon}, n^{2}_{\epsilon}) = (-v^2, v^1 + v^2).
\] (4)

We can check this as follows: Suppose a defect \( \mathbf{N} \) on a certain site in, say \( \Lambda_c \). Then, the vorticities counted by \( \varphi_k \) in \( \Lambda_c \) and in \( \Lambda_h \) are labeled as \( v^1 \) and \( v^2 \), respectively. On one hand, they also represent the discontinuities \( (e^1 + e^2) \cdot \mathbf{N} = n^1 + n^2 \) and \( -e^1 \cdot \mathbf{N} = -n^1 \), respectively. Therefore, we can see that equation (4) reproduces the vorticities located on the site; we shall provide some typical defect configurations observed in our MC simulations below.

Another key quantity is the helicity modulus defined as the response of the free energy against a long-wave-length (\( \lambda \)) twist of local order fields, which is proportional to the square of the wave number \( q \equiv 2\pi/\lambda \), i.e., \( \Upsilon(T) \equiv \lim_{q 
rightarrow 0} \partial^2 f(T, q)/\partial q^2 \) [9]. For the present model, the twist can be imposed by, for instance, \( \forall \ l \in \Lambda_h: \varphi_l \rightarrow \varphi_l + \mathbf{q} \cdot \mathbf{x}_l \) and \( \forall \ m \in \Lambda_c: \varphi_m \rightarrow \varphi_m - \mathbf{q} \cdot \mathbf{x}_m \), where \( \mathbf{x}_l (\mathbf{x}_m) \) is the position vector of the \( l \)th \( (m \)th) site, and \( \mathbf{q} \equiv q/\Omega \) is the unit vector in the \( x \) direction of the basal 2D space. Then, one finds the following expression:

\[
\Upsilon(T) = \left\langle -\frac{1}{2} H - \frac{1}{T} \left( \sum_{(klm)} \sin(\varphi_k + \varphi_l + \varphi_m) \mathbf{q} \cdot \mathbf{x}_{lm} \right)^2 \right\rangle,
\] (5)

where \( \Omega \) is the 2D volume of the system [7]. While this is useful for MC simulations, its theoretical expression is also obtained as follows. From equation (3), the above twist can be
related to a shift in the vector field: $\Phi(x) \rightarrow \Phi(x) + q \cdot x(-e_1 + e_2)$. It then brings about the increase of the Gaussian part in the free energy density $(TK/2\pi)(q^2/2)$ [see equation (2)].

For $T \leq T_c$, we can renormalize effects of the defects, so that the helicity modulus in the full theory is given by $\Upsilon(T) = TK(l=\infty)/2\pi$. As usual, the ratio $\pi \Upsilon(T)/2T$ exhibits an universal jump from 1 to 0 at $T = T_c$ in the thermodynamic limit [7]. In the following MC simulation calculations, we shall use this criterion to determine the phase transition temperature.

**MC simulations and results.**—We shall provide MC data of the spin-spin correlation function and the helicity modulus. Through out our simulations, we used the standard Metropolis algorithm. First, we consider a long-rectangular system, i.e., $48 \times 480$-site system with periodic boundary conditions. This is because the critical spin-spin correlation function in the strip of $L \times \infty$ behaves as $C_L(x) = (S_k S_l) \propto [(L/\pi) \sin(\pi x/L)]^{-\eta}$ along the $x$ direction with the period $L$ [10]. Thus, also for the strip-like system above, we can expect a clear observation of the power-law decay with respect to the scaled variable $\sin(\pi x/L)$. The right panel of figure 1 exhibits log-log plots of $C_{48}(x)$ at four temperatures. Note that, in units of the lattice constant $a = 1$, the condition $x = 0 \pmod{3}$ should be satisfied to give nonvanishing correlations. We find the power law at $T = 0.7, 0.8,$ and $0.9$ while it deviates from the law, and may exhibit an exponential decay at $T = 1.0$. Also, to give an intuitive description on the role of the defects, we draw snapshots of some typical defect configurations in the left four panels, where a rectangular area including only $48 \times 48$ spins is exhibited. The primitive vectors are taken as $e_1 = (1,0)$ and $e_2 = (1/2, \sqrt{3}/2)$ using the frame as the Cartesian coordinate. At low temperature, we only observe a few number of small aggregations of defects, which thus hardly change the properties of the correlation. With the increase of temperature, the size and the number of aggregations become larger, and at $T = 1.0$ we can find them everywhere, which largely disturb the correlation, and then brings about the exponential decay observed. Therefore, we can conclude that the phase transition is driven by the topological defects and it takes place in between $T = 0.9$ and $1.0$.

Next, we give MC data of the helicity modulus. The $L \times L$ systems of sizes up to $L = 384$
were treated. $10^7$ MC steps (MCS) were used for samplings after $10^6$ MCS for equilibration. At each temperature, we performed independent runs up to 64 so as to attain reliable statistics of data. In units of $a = 1$, $\Omega = L^2/\zeta$, where $\zeta (= 2/\sqrt{3})$ is the geometric factor of $\Lambda$. Then, we obtain the helicity modulus which is given in figure 2 (the $L = 384$ case). As expected, it exhibits a steep decrease and crosses the straight line $2T/\pi$, from which a finite-size estimate of the transition temperature $T_c(L)$ is obtained. The inset gives an extrapolation of $T_c(L)$ to the thermodynamic limit. According to reference [7], we use an extrapolation formula, $T_c(L) = T_c(\infty) + c_1/(\ln L + c_2)^{1/\bar{\nu}}$, where $T_c(\infty)$ and $c_{1,2}$ are least-squares-fitting parameters, and $\bar{\nu} (= 3/5)$ is the exponent of the correlation length in the disordered phase. Then, we obtain $T_c(\infty) \simeq 0.905$, which agrees with the rough estimation based on the correlation function data.

Summary.—We have studied the defect-mediated phase transition observed in the triangular-lattice three-spin interaction model. It is similar to the BKT transition, but it is described by the vector sine-Gordon field theory. Based on it, we have discussed properties of the phase transition, the spin-spin correlation functions and the temperature dependence of the helicity modulus. These arguments have been checked by the use of the large-scale MC simulations, and then we have clarified the phase transition quantitatively. On the other hand, one of the remaining questions is, for instance, whether our model and the phase transition above is realized in real materials or not. We will address these issues in future study.

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