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Phase Transitions in the Generalized XY Model at $f = 1/2$

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We numerically investigate the phase transitions in the generalized XY model at the frustration $f = 1/2$, in which the cosine interaction term in the original XY model is extended to the form $V^{(p)}(\theta) = E_J(2/p^2)[1 - \cos^{2p^2}(\theta/2)]$ with the gauge-invariant phase difference θ and the coupling strength E_J. As either the temperature T or the parameter p in the interaction potential is decreased, the Z_2 symmetry related with the two degenerate ground states of the original fully-frustrated XY model, corresponding to $p = 1$, is spontaneously broken at T_{Z_2}. The quasi-long-range order related with the $U(1)$ symmetry is detected from the helicity modulus, from which the transition temperature $T_{U(1)}$ is determined. The phase diagram in the (T, p) plane with phase boundaries for T_{Z_2} and $T_{U(1)}$ is constructed via Monte-Carlo calculations. As p is increased at low temperatures, a nonmonotonic behavior of the helicity modulus with a cusp-like structure is revealed when the ground state changes at $p_c = \sqrt{\ln(3/4)/\ln(\cos(\pi/8))/2} \approx 1.3479$.

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I. INTRODUCTION

The XY model has been introduced as an extension of the Ising model in which the planar spins of unit lengths are described by the angle variables with respect to some space-fixed direction. Not only does the XY model have a real-world example in the magnetic spin systems with the z-component of the spins suppressed but it can also successfully describe superconducting systems with an angle variable corresponding to the phase of the complex Ginzburg-Landau order parameter [1]. In the early seventies, the XY model in two dimensions (2D) was known to exhibit a very interesting critical behaviors, and its phase transition was well understood from the pioneering works by Kosterlitz and Thouless (KT) [2]. Different from other usual continuous transitions, the KT transition is characterized by the absence of a long-range order even in the low-temperature phase, but the correlation function decays algebraically at any temperature below the KT transition at $T_{U(1)}$ so that the term "quasi-long-range-order" well captures the peculiar order in the low-temperature region.

The two-dimensional Josephson junction array has often been studied as an experimental realization of the XY model [3,4]. In the presence of an external magnetic field $\boldsymbol{B}$ [5], the phase difference θ_{ij} across the Josephson junction between the two superconducting islands i and j is written in the gauge-invariant form $\theta_{ij} = \phi_i - \phi_j - A_{ij}$, where ϕ_i is the phase of the superconducting order parameter at site i. The magnetic bond angle A_{ij} is written as the line integral from i to j:

$$A_{ij} = \frac{2\pi}{\Phi_0} \int_i^j \boldsymbol{A} \cdot d\boldsymbol{l}$$

with the magnetic flux quantum Φ_0 for Cooper pairs and the magnetic vector potential $\boldsymbol{A}$. The use of the Landau gauge $\boldsymbol{A} = Bx\hat{\boldsymbol{y}}$ leads to $A_{ij} = 2\pi f x_i$ for $j = i + \hat{\boldsymbol{y}}$ and 0 for $j = i + \hat{\boldsymbol{x}}$ (the lattice constant is set to unity henceforth) [6], where the frustration f is defined as the number of flux quanta per plaquette, *i.e.*, $f = Ba^2/\Phi_0$. In the presence of an external magnetic field corresponding to the frustration f, the Hamiltonian of the frustrated XY model reads

$$H = -E_J \sum_{\langle ij \rangle} \cos(\theta_{ij} \equiv \phi_i - \phi_j - A_{ij}), \tag{1}$$

where E_J is the coupling strength and A_{ij} satisfies $\sum_{ij\in\alpha} A_{ij} = 2\pi f$ with the directional sum of four magnetic bonds around the plaquette α in the counter-clockwise direction. When $f = 1/2$, the magnetic bond angle takes values of either π or 0, and the ground state of the unfrustrated ($f = 0$) XY model [7] with $\phi_i =$

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const. cannot be the ground state of the fully-frustrated XY model ($f = 1/2$).

The phase transitions of the fully-frustrated XY (FFXY) model have been intensively studied for years [8]. First of all, the unique symmetry property of the FFXY model, namely the existences of Z_2 symmetry together with $U(1)$ symmetry, has been the origin of controversy. As more and more numerical and theoretical understanding have been made, there is now almost settled agreement among researchers that there are, indeed, well-split double transitions, at each of which the above-mentioned symmetry is broken one by one.

In this work, we generalize the FFXY model to allow an additional parameter called p [9], and we numerically investigate the phase transitions, with more focus put on the nonmonotonic behavior of the helicity modulus as p is varied. At low enough temperatures, we found that the helicity modulus Υ exhibited a cusp-like structure as a function of p, which became weaker at higher temperature. Eventually, the cusp-structure vanished as we crossed the critical point at (T_c, p_c).

The present paper is organized as follows: We first introduce our generalized XY model in Sec. II, and discuss the ground states configurations in Sec. III, which is followed by the presentation of our main results in Sec. IV. Finally, we summarize our main findings as a phase diagram in Sec. V and discuss the cusp-like structure in the helicity modulus.

II. GENERALIZED FULLY-FRUSTRATED *XY* MODEL

Within the resistively-shunted-junction formulation, the dynamic equations of motion of Josephson-junction arrays are obtained from the current conservation equations combined with the two Josephson relations, one for the supercurrent and the other for the voltage drop across the junction. The current conservation equation takes the form of the Langevin equation, with the thermal noise current included. Via the standard method to get the Fokker-Planck equation from the Langevin equation, one can obtain the stationary-state solution of the probability distribution function in the form of the Boltzmann distribution $\exp(-H/k_B T)$, which results in the XY Hamiltonian.

Alternatively, one can take the Ginzburg-Landau (GL) free-energy functional formulation to reach the same XY Hamiltonian. In more detail, the GL free energy H_{GL} for the complex order parameter $\Psi(\boldsymbol{r})$ is written in the following form [10]:

$$H_{GL} = \int d\boldsymbol{r} \left[\alpha |\Psi(\boldsymbol{r})|^2 + \frac{\beta}{2} |\Psi(\boldsymbol{r})|^4 + \frac{1}{2m^*} \left| \left(\frac{\hbar}{i} \nabla - \frac{q^*}{c} \boldsymbol{A} \right) \Psi(\boldsymbol{r}) \right|^2 \right], \quad (2)$$

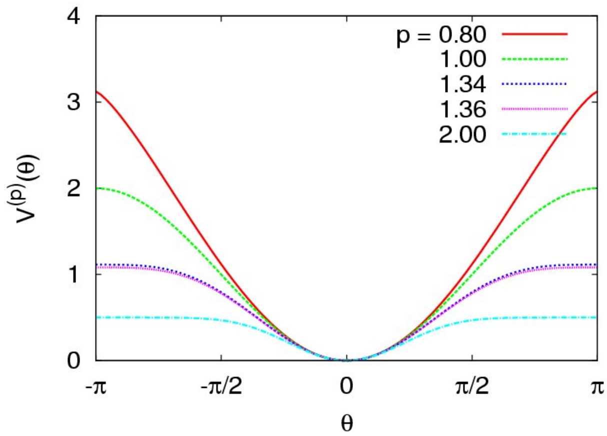

Fig. 1. Generalized potential $V^{(p)}(\theta)$ as a function of the gauge-invariant phase difference θ. At $p = 1$, the original cosine interaction of the XY Hamiltonian is recovered. As $\theta \to 0$, the quadratic form ($\sim\theta^2$) is confirmed, regardless of the values of p.

where m^* and q^* are the mass and the charge of a Cooper pair, respectively, We discretize the integral on a two-dimensional square grid structure and neglect the amplitude fluctuation taking the phase-only-approximation. Interestingly, the resulting form is the XY Hamiltonian, but with the approximation $\cos\theta \approx 1 - \theta^2/2$ taken for $\theta \ll 1$. In this regards, the discretized GL formulation makes it legitimate to use any interaction form $V(\theta)$ as long as the following two conditions are fulfilled: (i) $V(\theta)$ must be periodic in θ with the period 2π and (ii) in the limit of $\theta \to 0$, $V(\theta) \propto \theta^2$ should be satisfied.

In this work, we use the following generalized form [9]:

$$V^{(p)}(\theta) = \frac{2E_J}{p^2} \left[1 - \cos^{2p^2}(\theta/2) \right], \quad (3)$$

which clearly satisfies the above requirements for the legitimate interaction form because $V^{(p)}(\theta) \approx (E_J/2)\theta^2$, as displayed in Fig. 1. We also note that the original XY Hamiltonian is recovered when $p = 1$ by using the identity $2[1 - \cos^2(\theta/2))] = 1 - \cos\theta$. We use p and T as control parameters in our generalized fully-frustrated XY (GFFXY) model in Eq. (3) and study phase transitions and critical behaviors in the (T, p) plane.

III. GROUND STATE CONFIGURATIONS

The GFFXY model is described by the Hamiltonian

$$H = \sum_{\langle ij \rangle} V^{(p)}(\theta_{ij}), \quad (4)$$

where the gauge-invariant phase difference is given by $\theta_{ij} = \phi_i - \phi_j - A_{ij}$ with A_{ij} corresponding to $f = 1/2$. At $p = 1$ for the usual FFXY model, the ground state has been known to be doubly degenerate. The four bonds (let us call them θ_k with $k = 1, 2, 3, 4$) surrounding each plaquette in the ground state for $p = 1$ have either $\theta_k = \pi/4$ or $\theta_k = -\pi/4$ for all k, each with the vorticity $+1$ and -1, respectively [5]. In these ground states, every second plaquette has vorticity $+1$ and -1, forming a checker-board-type configuration. The double degeneracy comes naturally from the fact that the 2D lattice can be covered by two different types of checker boards with black and white interchanged. During our Monte-Carlo simulations, we find that these ground states at $p = 1$ are destroyed as p becomes larger and that the phase differences around a given plaquette are not $\pm\pi/4$ as for $p = 1$, but instead, three of them are 0, and the other remaining one is π: *e.g.*, $\theta_1 = \theta_2 = \theta_3 = 0$ and $\theta_4 = \pi$. The change in the ground state as p is varied is easily understood: The checker-board-type ground state is characterized by the bond energy $V^{(p)}(\theta) = V^{(p)}(\pm\pi/4)$ for all four bonds in a plaquette while the other ground state we observed has, *e.g.*, $V^{(p)}(\theta_1) = V^{(p)}(\theta_2) = V^{(p)}(\theta_3) = 0$ and $V^{(p)}(\theta_4) = V^{(p)}(\pi)$. Accordingly, the critical value of p_c is found from $V^{(p_c)}(\pi/4) = V^{(p_c)}(\pi)/4$, which gives us

$$p_c = \sqrt{\frac{\ln(3/4)}{\ln(\cos(\pi/8))/2}} \approx 1.3479. \qquad (5)$$

IV. MONTE-CARLO SIMULATIONS AND RESULTS

We perform the Monte-Carlo (MC) simulations through the use of the standard Metropolis algorithm with the local update rule. For convenience, the phase angles are discretized by 360 integer degrees, and at each value of p, we start from high temperatures and decrease the temperature slowly, storing the phase configuration at each temperature for the next run. Typically, more than 10^8 MC steps are used to compute the ensemble averages of various quantities, like the helicity modulus and the staggered vorticity [11].

The helicity modulus Υ is defined as the second-order stiffness of the free energy upon a twist δ of the phase angles across the system. More specifically, the free energy difference with and without δ is written as $\Delta F = \Upsilon(\delta^2/2) + \Upsilon_4(\delta^4/24)$ with the helicity modulus Υ and the fourth-order modulus Υ_4 [12]. The KT transition is conveniently detected by using the helicity modulus: Υ is finite at $T < T_{U(1)}$ because the quasi-long-range order makes the system stiff upon the twist while $\Upsilon = 0$ at $T > T_{U(1)}$ where phases are uncorrelated. Exactly at $T_{U(1)}$, the helicity modulus has been shown to make a jump from zero to a universal value $(\pi/2)T_{U(1)}$ [13] as T is decreased, which has been used as a way to determine $T_{U(1)}$ precisely.

In Fig. 2(a), we show Υ as a function of T at $p = 1.0$. In order to determine $T_{U(1)}$, we apply the universal jump condition as follows [see Fig. 2(b)]: (i) Find the crossing

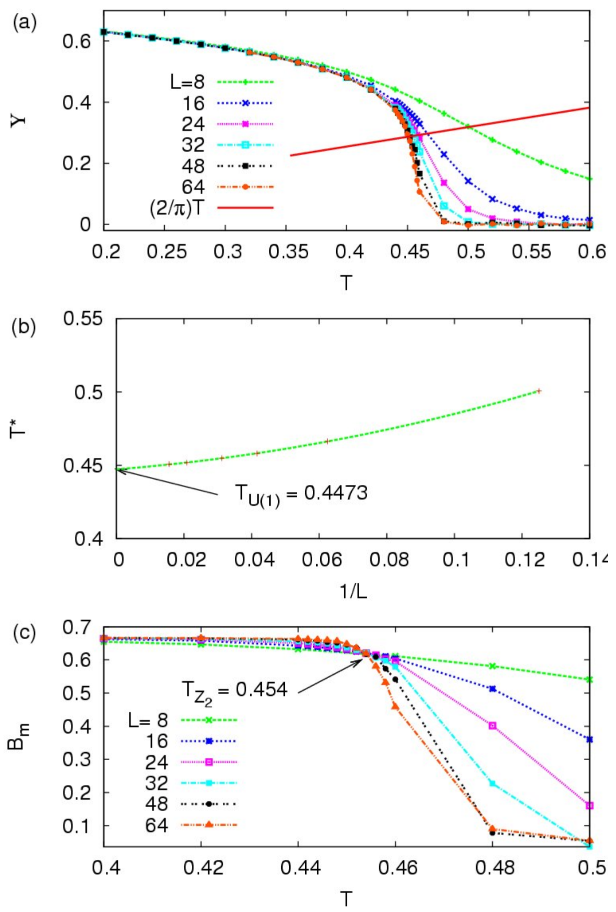

Fig. 2. (a) Helicity modulus Υ as a function of the temperature T at $p = 1.0$. In (b), we display how the estimate of $T_{U(1)}$ in the thermodynamic limit is made via the extrapolation. (c) Binder's cumulant for the staggered vorticity crosses at T_{Z_2}.

point $T^*(L)$ satisfying $\Upsilon(T^*) = (2/\pi)T^*$ for each system size L. (ii) Plot $T^*(L)$ as a function of $1/L$ and make an extrapolation towards $1/L \to 0$ via curve-fitting to a second-order polynomial to get an estimate of $T_{U(1)}$ in the thermodynamic limit. The critical temperature found in this way is $T_{U(1)} \approx 0.447$ for $p = 1$, which is in a good agreement with finding in Ref. 14 $T_{U(1)} \approx 0.446$.

The Ising-type order related with the Z_2 symmetry of the doubly-degenerate checker-board ground states is easily measured by using the staggered vorticity, analogous to the staggered magnetization of the antiferromagnetic Ising model. For $p < p_c$, the Ising-type order is destroyed either as T is increased or p is increased beyond p_c. However, the driving mechanism behind the transition is very different. When T is increased at fixed p below p_c, thermal fluctuation makes the checker-board-type ground states disordered. In contrast, as p is increased at fixed T, the vanishing of the order parameter is not related with any fluctuation, but simply results from a change in the ground states. From this reasoning, the phase boundary splitting two phases with $m = 0$

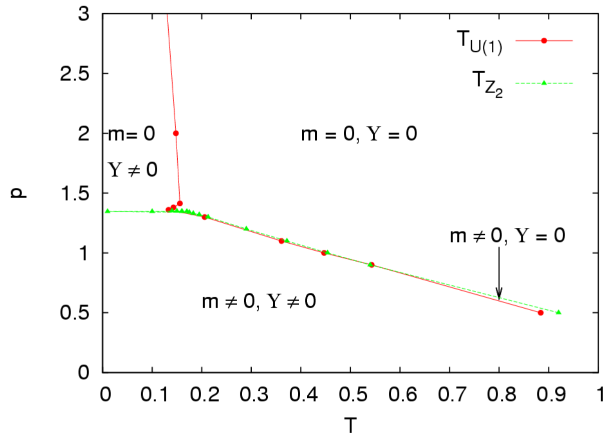

Fig. 3. Phase diagram of the generalized fully-frustrated XY model in the (T, p) plane. Two phase boundaries, one for the phase rigidity and the other for the Ising order, split the plane into four different regions.

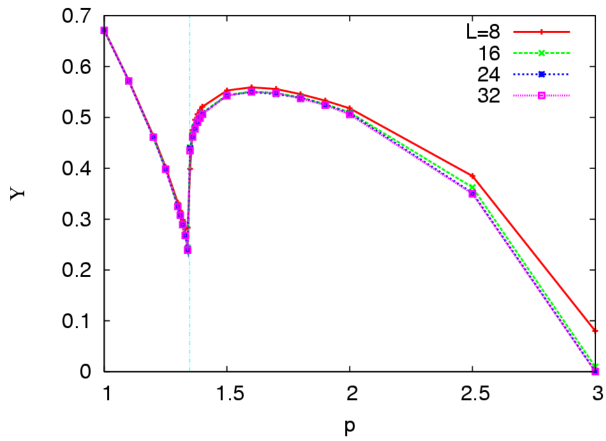

Fig. 4. Helicity modulus Υ at $T = 0.1$ as a function of p. As p is increased, Υ shows a nonmonotonic behavior with a cusp-like structure at $p = p_c$.

and $m \neq 0$ is expected to start from $(T = 0,\ p = p_c)$ and to extend as a horizontal line in the (T, p) plane up to (T_c, p_c). Below p_c, the Z_2 transition is conveniently captured by the Binder's cumulant [15], as is displayed in Fig. 2(c) for $p = 1.0$.

V. SUMMARY

We summarize our findings in the phase diagram in Fig. 3. Different from the usual FFXY at $p = 1$, a phase with phase stiffness ($\Upsilon \neq 0$), but without the Ising order of staggered magnetization ($m = 0$), is found to exist for $p > p_c$. Another interesting observation one can make from the phase diagram is that the separation of the two transition temperatures $T_{U(1)}$ and T_{Z_2} becomes larger as p is decreased. We also show the nonmonotonic behavior of the helicity modulus at $T = 0.1$ as a function of p in Fig. 4. As p is increased, Υ first decreases and then begins to increase again as p passes p_c. However, since $\Upsilon(T = 0.1, p_c)$ does not vanish, the system remains quasi-long-range-ordered. Although not shown here, $\Upsilon(T, p_c)$ is found to decrease as T is increased and eventually to vanish as we cross $T_c \approx 0.16$.

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