

Phase transitions in XY antiferromagnets on plane triangulations

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Using Monte Carlo simulations and finite-size scaling, we investigate the XY antiferromagnet on the triangular, Union Jack, and bisected-hexagonal lattices, and in each case find both Ising and Kosterlitz-Thouless transitions. As is well known, on the triangular lattice, as the temperature decreases the system develops chiral order for temperatures $T < T_c$, and then quasi-long-range magnetic order on its sublattices when $T < T_s$, with $T_s < T_c$. On the Union Jack and bisected-hexagonal lattices, by contrast, we find that as T decreases the magnetizations on some of the sublattices become quasi-long-range ordered at a temperature $T_s > T_c$, before chiral order develops. In some cases, the sublattice spins then undergo a second transition, of Ising type, separating two quasi-long-range ordered phases. On the Union Jack lattice, the magnetization on the degree-4 sublattice remains disordered until T_c and then undergoes an Ising transition to a quasi-long-range ordered phase.

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I. INTRODUCTION

Two-dimensional fully frustrated XY (FFXY) models have been the subject of considerable interest over the past three decades; for a recent review see Ref. 1. In addition to their intrinsic theoretical importance within the field of critical phenomena, such models can also be realized experimentally via Josephson junction arrays (JJAs) in a uniform magnetic field.^{2,3}

In this work, we provide strong numerical evidence that the magnetic transitions of FFXY models can display rather unusual behavior. In particular, we observe a magnetic transition from disorder to quasi-long-range order which is in the Ising universality class, rather than the Kosterlitz-Thouless class, as would be expected for two-dimensional XY models.

On the triangular lattice, or indeed any triangulation of the plane, the FFXY model coincides with the usual antiferromagnetic XY (AFXY) model,^{4,5} defined by the reduced Hamiltonian

$$\mathcal{H} = J \sum_{ij} \mathbf{s}_i \cdot \mathbf{s}_j = J \sum_{ij} \cos(\theta_i - \theta_j), \quad (1)$$

where $\mathbf{s}_i = (\cos \theta_i, \sin \theta_i)$ is a planar spin with unit length on lattice site i , $J = 1/T$ is the inverse temperature, and the summation is over all nearest-neighbor pairs of sites.

The ground states of the triangular-lattice AFXY model are such that the spins on each of the three equivalent triangular sublattices are perfectly aligned, with adjacent spins differing by an angle $\pm 2\pi/3$. In addition to an $SO(2)$ rotational degeneracy, generic of XY models, there is a discrete $\mathbb{Z}_2 \cong O(2)/SO(2)$ reflection degeneracy, induced by frustration, corresponding to the two possible *chiralities* of each elementary triangular face. The chirality of a face refers to the sign of the rotation of the spins as one traverses the face counterclockwise (see Fig. 1). At positive temperatures, the Mermin-Wagner theorem⁶ forbids the sublattice spins from ordering. However, for low temperatures, the sublattice magnetizations exhibit quasi-long-range (QLR) order (alge-

braically decaying correlations), while the chiral degrees of freedom exhibit a genuine long-range order.

Despite some early controversy,^{4,5,7-11} there is now a consensus^{1,12-19} that for a number of FFXY models sharing the same ground-state degeneracies, including the triangular-lattice AFXY model and square-lattice FFXY model,²⁰⁻²² the phase transition associated with the magnetic order parameter occurs at a temperature T_s strictly below the transition point T_c for the chiral order parameter. It is generally accepted¹ that the sublattice magnetizations disorder via a standard Kosterlitz-Thouless (KT) transition,²³⁻²⁵ while the chiralities undergo an Ising transition. The behavior $T_s < T_c$ is supported by theoretical arguments based on the unbinding of kink-antikink pairs.^{17,26}

In this work, we study the AFXY model on the Union Jack (UJ) and bisected-hexagonal (BH) lattices using Monte Carlo simulations and finite-size scaling. The UJ and BH lattices are plane triangulations that share many of the properties of the triangular lattice (see Fig. 1). In particular, the ground-state degeneracies of the AFXY model on each of these three lattices are identical. However, as we show, the critical behavior of the AFXY model on the UJ and BH lattices is qualitatively different from the triangular-lattice case. One concrete difference is that on both the UJ and BH lattices we find $T_s > T_c$. Similar behavior has been previously observed in uniformly frustrated XY models^{27,28} with less than full frustration.

Like the triangular lattice, the UJ and BH lattices are tripartite; each consists of three independent sublattices, which we label A , B , C . Since each sublattice is regular, we use a subscript to indicate its coordination number. The triangular lattice consists of sublattices A_6 , B_6 , and C_6 , UJ consists of A_4 , B_8 , C_8 , and BH consists of A_4 , B_6 , C_{12} (see Fig. 1). Unlike the triangular lattice, the sublattices of the UJ and BH lattices are not all equivalent, and this leads to interesting new physics.

On the UJ lattice, we find that the spins on the A_4 sublattice become QLR ordered at a different temperature to the spins on the B_8 and C_8 sublattices. Analogous behavior has very recently been observed in the four-state Potts

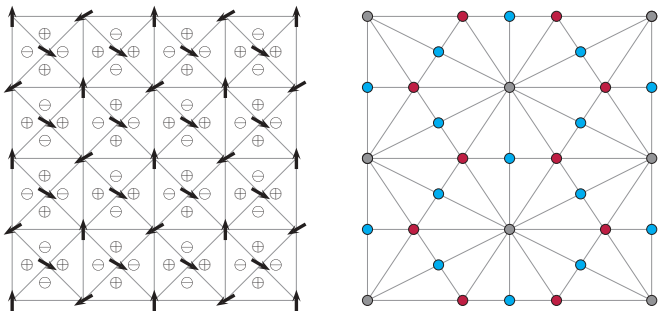


FIG. 1. (Color online) (Left) A ground-state configuration of the AFX model on the UJ lattice. The symbols + and - denote the chirality of the elementary triangular faces. (Right) A BH lattice. The tripartition of the vertex set is shown in purple/cyan/gray.

antiferromagnet.^{29,30} Perhaps more surprisingly, the magnetic transition of the A_4 spins, separating the disordered and QLR-ordered phases, appears to be an Ising transition. Such novel Ising transitions leading to QLR order, rather than genuine long-range order, have very recently been observed³¹ in generalized XY models whose Hamiltonians contain nematiclike interactions.^{31–34} Our study presents strong evidence that such transitions can in fact arise in the standard XY antiferromagnet.

II. SUMMARY OF RESULTS

A summary of the qualitative behavior of each lattice is presented in Fig. 2. On each lattice we observe a chiral transition at a temperature $T = T_c$, with $T_c(\text{Tri}) > T_c(\text{UJ}) > T_c(\text{BH})$. In each case we find strong evidence that the chiral transition is in the Ising universality class. In addition, in each case we also observe magnetic spin transitions at a temperature $T_s \neq T_c$, with $T_s(\text{Tri}) < T_s(\text{UJ}) < T_s(\text{BH})$. The qualitative features of the magnetic transition are highly lattice-dependent, however. On the triangular lattice, we observe a magnetic transition from disorder to QLR order on each of the three equivalent sublattices at $T_s > T_c$. The transition is consistent with the KT universality class.

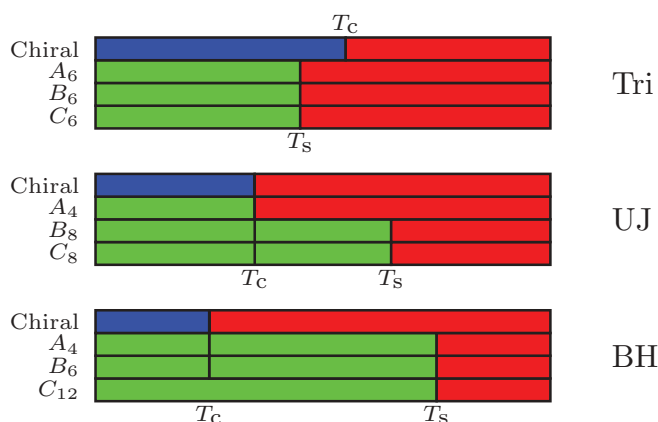


FIG. 2. (Color online) Summary of phases and transitions for AFX model on triangular (Tri), Union Jack (UJ), and bisected-hexagonal (BH) lattices. Red refers to disorder, blue to order, and green to QLR order. Temperature increases from left to right.

On the UJ lattice, we observe that the spins on sublattices B_8 and C_8 undergo a transition from disorder to QLR order, which is again consistent with KT behavior. However, on the UJ lattice, we find very clear evidence that $T_s > T_c$. Furthermore, we find no evidence of a spin transition on the A_4 sublattice at T_s , but we find strong evidence that the spins on the A_4 sublattice undergo an Ising transition from disorder to QLR order at (or extremely close to) T_c . In addition, it appears that the spins on the B_8 and C_8 sublattices undergo a second transition at T_c , which separates two QLR-ordered phases. This second transition appears to be in the Ising universality class, but the measured magnetic exponent takes a non-Ising value of 1.94(1).

On the BH lattice, the spins on each sublattice A_4 , B_6 , and C_{12} appear to transition from disorder to QLR order at a common value of $T_s > T_c$. The transition appears to be consistent with the KT universality class. The spins on A_4 and B_6 then undergo a second transition, consistent with the Ising universality class, at $T = T_c$, while the spins on C_{12} do not. The C_{12} sublattice appears to display generic KT behavior.

III. MONTE CARLO SIMULATIONS

Our simulations used a local algorithm based on a mixture of standard local Metropolis³⁵ updates together with over-relaxed^{36,37} (microcanonical) updates. Periodic boundary conditions are applied, and the maximum linear system size is $L_{\max} = 384,256$, and 256 for the triangular, UJ, and BH lattices, respectively. The total CPU time for the simulations was approximately 60 years, with a 3.2-GHz Xeon EM64T processor.

For each sublattice $S = A, B, C$, we define the magnetic order parameter $\mathbf{M}_S = (1/V_S) \sum_{i \in S} \mathbf{s}_i$, with $V_S = |S|$. The chiral order parameter is defined as

$$M_c = \frac{2}{3\sqrt{3}N_\Delta} \sum_{\Delta} [\sin(\theta_i - \theta_j) + \sin(\theta_j - \theta_k) + \sin(\theta_k - \theta_i)],$$

where the summation is over the N_Δ triangular faces. The sequence (i, j, k) is alternately chosen clockwise and counterclockwise on neighboring triangles. The magnetic and chiral susceptibilities are then defined to be $\chi_S = V_S \langle M_S^2 \rangle$ and $\chi_c = N_\Delta \langle M_c^2 \rangle$, and we also define dimensionless ratios $Q_S = \langle M_S^2 \rangle^2 / \langle M_S^4 \rangle$ and $Q_c = \langle M_c^2 \rangle^2 / \langle M_c^4 \rangle$. These ratios, which are closely related to the Binder cumulant,³⁸ have been well-studied for both the Ising and XY universality classes, and accurate estimates of their values are available.^{39–41} In addition, on each sublattice S , we measure the nearest-neighbor spin-spin correlation function E_S and define a specific-heat-like quantity $C_S = V_S(\langle E_S^2 \rangle - \langle E_S \rangle^2)$. While the quantities C_S may not be physically measurable, they are convenient theoretical devices for studying critical behavior.

A. Triangular lattice

As T decreases, the Q_c data for different system sizes display an approximately common intersection near $T \approx 0.512$. For $T \lesssim 0.512$, the Q_c value quickly approaches 1, and $\langle M_c^2 \rangle$ converges to a nonzero value as L increases, implying the occurrence of chiral order. The spins on the three sublattices remain disordered until $T \approx 0.50$, where the Q_S data indicate a

magnetic transition on each of the three equivalent sublattices $S = A_6, B_6, C_6$. In the low-temperature region $T \lesssim 0.50$, as L increases, the Q_S data converge to a line of nontrivial T -dependent values, implying that each sublattice is QLR ordered.

For small $\Delta_c = T - T_c$, the ratio Q_c is expected to behave like

$$Q_c = Q_c^* + a_1 \Delta_c L^{y_t} + a_2 \Delta_c^2 L^{2y_t} + b/L, \quad (2)$$

where a_1 , a_2 , and b are free parameters, and $y_t = 1/\nu$ is the leading thermal renormalization exponent. We performed least-squares fits of (2) to the Q_c data near $T \approx 0.512$. The data with $L \geq 24$ are well described by (2), and the fit yields $T_c = 0.5123(2)$, $y_t = 0.99(1)$, and $Q_c^* = 0.8587(3)$.

We also performed least-squares fits of the χ_c data to

$$\chi_c = L^{2y_h-2} (a_0 + a_1 \Delta_c L^{y_t} + a_2 \Delta_c^2 L^{2y_t} + b/L), \quad (3)$$

with the fixed Ising value $y_t = 1$. This yields a critical point $T_c = 0.5123(1)$ and magnetic exponent $y_h = 1.874(3)$.

The estimated critical exponents, $y_t = 0.99(1)$ and $y_h = 1.874(3)$, agree well with the exact results $y_t = 1$ and $y_h = 15/8$ for the two-dimensional Ising model. The critical value $Q_c^* = 0.8587(3)$ is also consistent with the existing result $Q_{\text{Ising}}^* = 0.85872528(3)$ for the ferromagnetic triangular-lattice Ising model.⁴⁰ We conclude that the chiral transition is in the Ising universality class. We note that our estimate of y_t is inconsistent with several earlier values reported in the literature^{15,19,42} which suggested $y_t \approx 1.2$. Our estimate of T_c is close to the recent estimate¹⁹ of $T_c = 0.51254(3)$.

Compared with the chiral transition, it is much more difficult to locate the spin transition of the sublattice magnetizations. It is known^{43,44} that at a KT transition the susceptibility diverges as $\chi \propto L^{7/4} (\ln L)^{1/8}$. Assuming that the spin transition is of KT type, we therefore consider the curves of $\chi_{A_6} L^{-7/4} (\ln L)^{-1/8}$ vs T for a number of fixed L . From the scaling of the intersections for various $24 \leq L \leq 384$ and $0.500 \leq T \leq 0.505$, we obtain $T_s = 0.5040(3)$. This value is consistent with the recent estimate¹⁹ of $T_s = 0.504(1)$.

B. Union-jack lattice

Figure 3 shows that for sufficiently low temperatures, the susceptibility on each sublattice displays an algebraic divergence with a temperature-dependent exponent, signifying a QLR-ordered phase precisely as observed on the triangular lattice. From Fig. 4, which plots $\chi_{B_8} L^{-7/4}$ and Q_{B_8} vs T , we see that the spins on the sublattice B_8 (and also C_8) undergo two distinct phase transitions, one at $T \approx 0.43$ and another at $T \approx 0.64$. By contrast, Fig. 5 shows that the spins on sublattice A_4 undergo a single transition near $T \approx 0.43$.

Assuming that the spin transition near $T \approx 0.64$ is a KT transition, the χ_{B_8} data were analyzed in an analogous manner to that described for the χ_{A_6} data on the triangular lattice. This yields an estimate of the spin transition point on the B_8 and C_8 lattices of $T_s = 0.639(2)$.

For the chiral transition, fitting the Q_c data to (2) analogously to the triangular case yields $T_c = 0.4316(1)$, $y_t = 0.99(1)$, and $Q_c^* = 0.8562(3)$. Similarly, fitting χ_c to (3) with $y_t = 1$ fixed yields $T_c = 0.4316(1)$ and $y_h = 1.874(3)$. Not only do these values of y_t and y_h agree with the known Ising

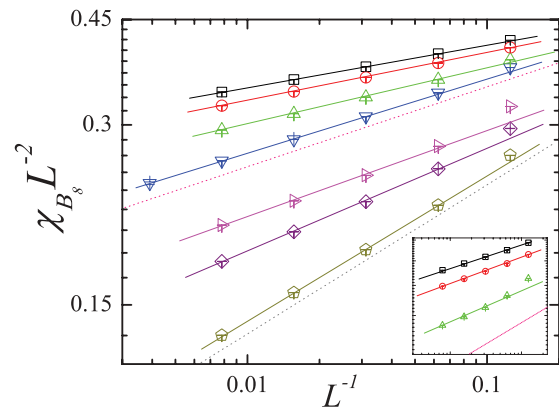


FIG. 3. (Color online) Log-log plot of $\chi_{B_8} L^{-2}$ versus L^{-1} on the UJ lattice. From top to bottom the solid lines correspond to temperatures $T \approx 0.357, 0.385, 0.417, 0.431, 0.5, 0.556, 0.633$. The inset shows the $\chi_{A_4} L^{-2}$ data for $T \approx 0.357, 0.385, 0.417$. The dotted lines correspond to the critical temperatures T_c and T_s .

values, but the estimated value of Q_c^* is also in excellent agreement with the existing estimate $Q_{\text{Ising}}^* = 0.8562157(5)$ for the square-lattice Ising model,^{39,40} as expected from the geometry of the UJ lattice. These results therefore provide strong evidence that the chiral transition is again in the Ising universality class.

Perhaps surprisingly, fitting the Q_{A_4} and χ_{A_4} data near $T \approx 0.43$ in a similar way also produces excellent fits, which yield $T_{A_4} = 0.4316(1)$, $y_t = 1.00(1)$, $y_h = 1.874(2)$, and $Q_{A_4}^* = 0.8563(4)$. This suggests two things. First, within the resolution of our simulations, the transition points of the A_4 and chiral transitions coincide, implying that either $T_{A_4} = T_c$ exactly, or that $|T_{A_4} - T_c| \lesssim 0.0001$. Secondly, and most strikingly, the critical behavior associated with the A_4 spin transition is consistent with the *Ising* universality class, rather than the KT universality class as one might have expected. This suggests that the magnetization on the A_4 sublattice undergoes an Ising transition from a disordered phase to a QLR-ordered phase at (or very close to) $T = T_c$. Further evidence supporting this claim is provided by the divergence of C_{A_4} at T_c , as shown in the inset of Fig. 6. Based on these observations, we make the rather remarkable conjecture that the A_4 sublattice spins

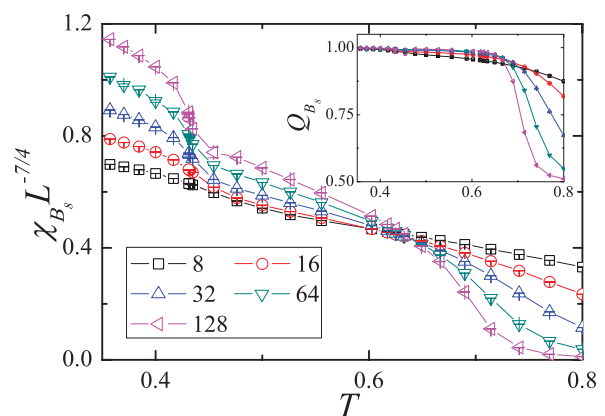


FIG. 4. (Color online) $\chi_{B_8} L^{-7/4}$ vs T for various L , on the UJ lattice. The inset shows Q_{B_8} vs T .

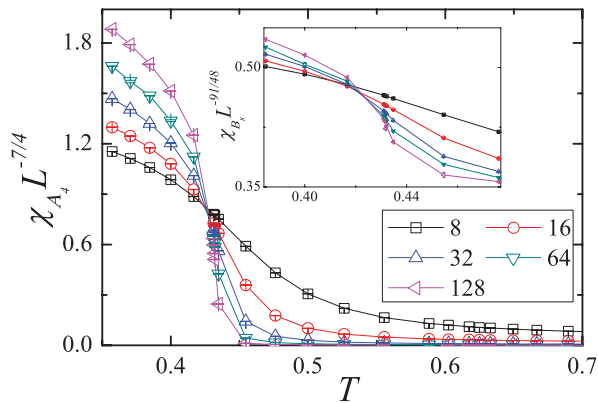


FIG. 5. (Color online) $\chi_{A_4} L^{-7/4}$ vs T for various L , on the UJ lattice. The inset shows $\chi_{B_8} L^{-91/48}$ vs T .

undergo an Ising transition precisely at the chiral transition temperature T_c .

In addition, we find that the spins on sublattices B_8 and C_8 also undergo a transition near (or at) T_c , in addition to the transition at $T_s > T_c$. Fitting the B_8 susceptibility data near T_c to (3) with both y_t and y_h free, we find a second B_8 transition at $T = 0.4316(4)$, with exponents $y_t = 1.00(1)$ and $y_h = 1.94(1)$. The estimate $y_t = 1.00(1)$ agrees perfectly with the exact Ising value $y_t = 1$, and the transition temperature is also entirely consistent with our estimate of the chiral transition temperature T_c . From Fig. 3, however, it is clear that the phases of the B_8 spins on either side of T_c are both QLR ordered. We therefore conjecture that at the chiral transition temperature T_c , the spins on the B_8 and C_8 sublattices undergo an Ising transition separating two QLR-ordered phases. This suggests that the chiral transition at T_c induces Ising transitions in the spins on each of the three sublattices; however the physical mechanism underlying this behavior remains to be determined.

As further evidence that the B_8 sublattice undergoes transitions at both T_s and T_c , Fig. 6 shows the specific-heat-like quantity C_{B_8} . We clearly observe a peak near T_s and a divergence near T_c as $L \rightarrow \infty$, consistent with KT and Ising behavior, respectively. For comparison, the inset shows C_{A_4} , which does not show any peak near T_s .

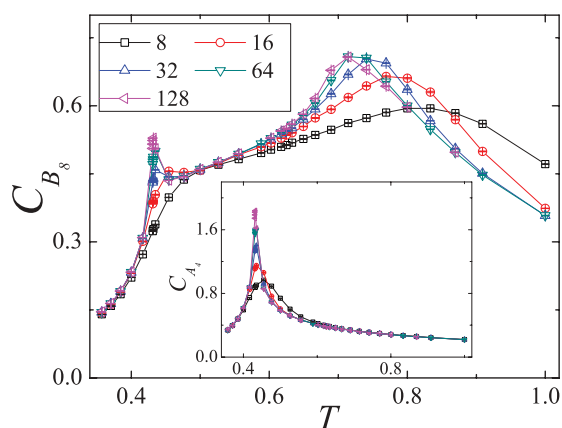


FIG. 6. (Color online) C_{B_8} versus T on the UJ lattice. The inset shows C_{A_4} .

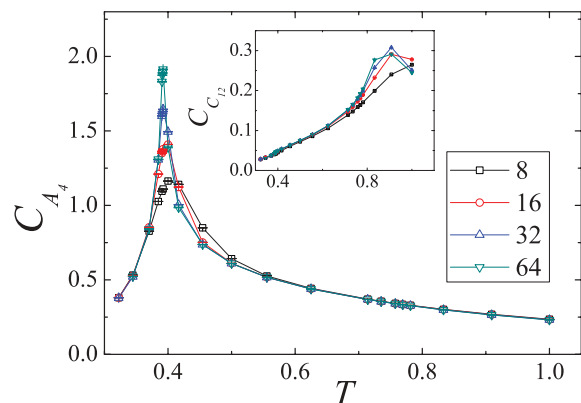


FIG. 7. (Color online) C_{A_4} versus T on the BH lattice. The inset shows $C_{C_{12}}$.

The value of $y_h = 1.94(1)$ is clearly not equal to the usual Ising value, and determining it exactly remains to be further explored. We remark, however, that it is numerically very close to the fractal dimension of critical Ising domains $\frac{187}{96} \approx 1.9479\dots$ ^{45,46} It is tempting to therefore conjecture that $y_h = 187/96$ exactly for the transition at T_c on the B_8 and C_8 sublattices. For illustration, the inset of Fig. 5 shows $\chi_{B_8} L^{-91/48}$ vs T .

C. Bisected-hexagonal lattice

Analyzing χ_c and Q_c in the same manner as for the triangular and UJ lattices, we find that the chiral order parameter undergoes an Ising transition at $T_c = 0.39137(8)$. Similarly, an analysis of the sublattice susceptibilities shows that the spins on each sublattice undergo a transition from disorder to QLR order at a common value of $T_s = 0.747(2)$. These magnetic transitions are again consistent with the KT universality class. As for the B_8 and C_8 sublattices on the UJ lattice, χ_{A_4} and χ_{B_6} show that the A_4 and B_6 sublattices of the BH lattice also undergo an Ising transition at $T = T_c$. Near T_c , the specific-heat-like quantities C_{A_4} and C_{B_6} are observed to be divergent for $L \rightarrow \infty$, while $C_{C_{12}}$ seems to be a smooth function. By contrast, near T_s , a peak occurs in $C_{C_{12}}$ which is absent in C_{A_4} and C_{B_6} (see Fig. 7). These observations suggest that the magnetic transition on C_{12} is a generic KT transition, and that the QLR magnetic order on A_4 and B_6 in the region $T_c \leq T \leq T_s$ is likely induced by the long-range correlation length on C_{12} .

IV. DISCUSSION

In this work, we have studied the XY antiferromagnet on three plane triangulations: the triangular, UJ, and BH lattices. Each of these lattices is tripartite. In each case we find that the chiral order parameter undergoes a standard Ising order/disorder transition. This behavior should be generic on all tripartite triangulations of the plane, since the set of ground states will share the same \mathbb{Z}_2 chiral degeneracy. However, as we have shown, the nature of the magnetic transitions appears to be strongly dependent on the specific lattice topology.

In addition to the intrinsic theoretical interest of these results, we note the AFX model on the UJ lattice could

be realized experimentally using Josephson junction arrays in an entirely similar manner to the triangular-lattice model. Therefore, the results that we have outlined above should be experimentally observable.

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