Nematic and chiral orders for planar spins on triangular lattice

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We propose a variant of the antiferromagnetic XY model on the triangular lattice to study the interplay between the chiral and nematic orders in addition to the magnetic order. The model has a significant bi-quadratic interaction of the planar spins. When the bi-quadratic exchange energy dominates, a large temperature window is shown to exist over which the nematic and the chiral orders co-exist without the magnetic order, thus defining a chiral-nematic state. The phase diagram of the model and some of its critical properties are derived by means of the Monte Carlo simulation.

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Nontrivial orders in frustrated magnets [1] are among the central issues in the field of condensed-matter physics. Besides the conventional magnetic order parameter of spin $S_i$ at a site $i$, there could appear various nontrivial orders such as vector [2, 3] and scalar [4, 5] chiral orders [6], and nematic order [7], which might lead to additional phase transitions distinct from the one driven by magnetic order. Even the ground state itself may be characterized solely by these nontrivial orders. This issue is now attracting revived interest from the viewpoint of nontrivial glass transition of spins [8] and multiferroic behaviors [9, 10], where the ferroelectricity is induced by the formation of vector spin chirality [11]. One important aspect of this problem is the interplay between the various orders. Usually the nontrivial orders become long ranged when the magnetic order sets in. For example, the spiral spin order naturally implies the vector spin chiral order through $(S_i \times S_j) \sim (S_i) \times (S_j)$ on the neighboring sites. Therefore, the interesting issue is whether the nontrivial order can become long ranged in the absence of the magnetic order. This issue has been studied theoretically [9], and experimentally in the quasi-one dimensional frustrated magnet [12] where the chiral order appears above the magnetic phase transition. The next important question, we argue, is the interplay between the two nontrivial orders, e.g., chiral and nematic orders, which has not been fully addressed so far.

To address this issue, we study a generalized classical XY spin model on a triangular lattice,

$$H = J_1 \sum_{(ij)} \cos(\theta_{ij}) + J_2 \sum_{(ij)} \cos(2\theta_{ij}),$$

(1)

where $\theta_{ij}$ is the angle difference $\theta_i - \theta_j$ between the nearest neighbors $\langle ij \rangle$. This model contains the usual frustration in the exchange interaction due to the triangular lattice geometry, together with the possible nematic order induced by the $J_2$ term. The $J_2 = 0$ limit has been extensively studied, and it is believed to have two phase transitions at closely spaced critical temperatures[2, 13–15]. The Kosterlitz-Thouless (KT) transition temperature $T_{KT}$ signaling the loss of (algebraic) magnetic order and the melting temperature of the staggered chirality, $T_C$, are extremely close, $(T_C - T_{KT})/T_C \lesssim 0.02$ at $J_2 = 0$, hampering the interpretation of the intermediate, $T_{KT} < T < T_C$ phase as the chiral phase in which the chirality is ordered but the magnetism remains disordered. Extension of the XY model to include large $J_2$ interaction was considered earlier in Refs. [16, 17], where the authors examined the phase diagram of Eq. (1) on the square lattice, which lacks frustration. In contrast, our model on the triangular lattice serves as a minimal model to study the two nontrivial orders, i.e., the chiral order induced by the geometric frustration, and the nematic order induced by the bi-quadratic interaction.

A unique feature of the large $J_2/J_1$ region of the model as noted in Refs. [16, 17] is the existence of an Ising phase transition associated with the vanishing string tension between half-integer vortices in addition to the KT transition. This Ising phase transition turns out to correspond to the onset of the (algebraic) magnetic order. Being driven by $J_1$, the Ising transition temperature occurs at a much lower temperature than either the chiral or the nematic transition, which are both driven by $J_2$. The result is the existence of a magnetism-free, chiral-nematic phase in the large $J_2/J_1$ part of our model.

Phase diagram: The $x-T$ phase diagram for Eq. (1) is shown in Fig. 1, where $T$ is the temperature and $x$ parameterizes the interaction as $J_1 = 1 - x$, $J_2 = x$. Detailed Monte Carlo (MC) calculations were performed with $5 \times 10^5$ MC steps per run, on $L \times L$ lattice with $L$ ranging from 15 to 60. Occasional checks were made on a larger lattice of up to $L = 100$ to ensure that no discernible changes in either the critical temperatures or the critical exponents are obtained from the larger size.
FIG. 1: (Color online) Phase diagram of the J$_1$−J$_2$ model in Eq. (1) with J$_1 = 1 − x$ and J$_2 = x$. Two closely spaced transition temperatures labeled by $T_{KT}$ and $T_x$ separate the paramagnetic (PM) phase from the algebraically correlated phase at a lower temperature, aM, aN, and C stand for phases with algebraic correlations in (antiferro)magnetic and (antiferro)nematic order parameters, and the long-range correlations in the chirality order. A further transition from aN to aM occurs as an Ising transition for $x > x_c$ with $x_c ≈ 0.7$. All the symbols have a thickness in the temperature direction consistent with their statistical errors. (inset) The onset of chirality order at $T_x$ (red) takes place at temperatures close to, but slightly higher than the corresponding KT transition temperature $T_{KT}$ (black) for all $x$. The Ising transition temperature $T_I$ is not shown here for clarity.

Typically, $10^5$ steps were discarded to reach equilibrium. An integer vortex-mediated KT transition marking the PM-aM boundary bifurcates into a half-integer vortex-mediated KT transition, marking the PM-aN boundary, plus an Ising transition [16] when $x$ exceeds $x_c ≈ 0.7$. The Ising transition in turn separates the aM from aN. For the whole range of $x$, the chiral transition temperature $T_x$ stays slightly above $T_{KT}$, with the possible exception at $x = x_c$ where they may coincide.

**KT transition at $T_{KT}$**: The determination of $T_{KT}$ is made with the phase stiffness, also called the helicity modulus, appropriate for the $J_1$−$J_2$ model

$$\rho_\phi(T) = -\frac{J_1}{2L^2} \left( \sum_{\langle ij \rangle} \cos \theta_{ij} \right) - \frac{2J_2}{L^2} \left( \sum_{\langle ij \rangle} \cos 2\theta_{ij} \right)$$

$$- \frac{1}{TL^2} \langle \sum_{\langle ij \rangle} x_{ij} \sin \theta_{ij} + 2J_2 \sum_{\langle ij \rangle} x_{ij} \sin 2\theta_{ij} \rangle^2. \quad (2)$$

Here $x_{ij} = x_i - x_j$ is the separation of the $x$-coordinate. The crossing of $\rho_\phi(T)$ with the straight line $(2/\pi)(\sqrt{3}/2)(J_1 + 4J_2)T = (2/\pi)(\sqrt{3}/2)(1 + 3x)T$ yields, for a given lattice size $L$, an estimate of the critical temperature $T_{KT}(L)$ [14]. Extrapolation to $L \to \infty$ using polynomial fits as shown in the insets of Fig. 2 yields the estimate of $T_{KT}$. A more sophisticated method taking into account the logarithmic correction [18] yields a similar answer [15].

**Chirality transition at $T_x$**: It is customary to define the chirality $\chi$ as the directed sum of the bond current $\langle \sin \theta_{ij} \rangle$ [13] following the relation $\langle \sin \theta_{ij} \rangle \sim -\partial F/\partial A_{ij}$. The free energy $F$ is evaluated with respect to the modified interaction $\cos \theta_{ij} \to \cos(\theta_{ij} + A_{ij})$. A similar modification of Eq. (1) results in the bond current

$$J_{ij} \sim J_1 \langle \sin(\theta_{ij}) \rangle + 2J_2 \langle \sin(2\theta_{ij}) \rangle. \quad (3)$$

This new definition is particularly effective as $x \to 1$, where the conventional definition $\sim \langle \sin \theta_{ij} \rangle$ vanishes identically due to the $Z_2$ symmetry. For each $x$, $T_x$ was obtained from Binder cumulant analysis for the new definition of chirality based on Eq. (3). The conventional definition $(J_2 = 0)$ gave an estimate of $T_x$ which differs only in the third significant digit. Although our analysis showed $T_x \gtrsim T_{KT}$ for all $x$, we do not at present rule out the scenario in which $T_x$ and $T_{KT}$ merge at $x = x_c$, resulting in a multi-critical point there. If that happens, the second-order chirality transition may become weakly first-order.

Earlier analysis [14] at $x = 0$ identified the transition of $\chi$ with the non-Ising critical exponents $1/\nu = 1.2$, and $\beta/\nu = 0.12$, $\gamma/\nu = 1.75$. Figure 3 shows $\chi$ and its variant, $\psi \equiv (\langle \chi^2 \rangle - \langle \chi \rangle^2)/\langle \chi \rangle$, in scaling form $\chi = L^{-\beta/\nu}f(tL^{1/\nu})$, $\psi = L^{\gamma/\nu}g(tL^{1/\nu})$, with $t = (T - T_x)/T_x$, at $x = 0.3$ and $x = 0.8$. Same exponents as for the $x = 0$ case works well in scaling throughout the whole phase diagram. Appearance of the non-Ising exponents for $J_2 = 0$ have been explained in terms of an enhanced finite-size scaling effect at small sizes due to the screening length associated with the KT transition, in the cases of the square lattice [13] and triangular lattice [14]. Here it is equally possible that the true universality classes at $T_x$ that of Ising transition. At any rate, the identification of the chirality transition $T_x$ well above the magnetic transition for large $J_2/J_1$ ratio is unequivocal and proves the existence of the magnetism-free, chiral-nematic phase in our model.

FIG. 2: (Color online) Phase stiffness $\rho_\phi(T)$ according to Eq. (2) for $L = 15$ − $60$ and $x = 0.5$ and $0.9$. The straight line is $(2/\pi)(\sqrt{3}/2)(J_1 + 4J_2)T$. The crossing temperature of this line and $\rho_\phi(T)$ for each $L$ is shown in the inset along with the extrapolation to $L^{-1} = 0$. 

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The last row shows the behavior of the Binder cumulants at $x = 0.3$ and $x = 0.8$, for lattice sizes $L = 15 - 60$. The exponents used are those of $x = 0.14$. The critical nature of the nematic order parameter $N$ at $x > x_c$ is seen in the continuous dependence of the exponent $\eta_N$, $N \sim 1/L^{\eta_N(T)}$, as shown in Fig. 4 (b) for $x = 0.9$. The $T$-dependent exponent $\eta_N(T)$ continuously decreases as the temperature is lowered, even in the low-$T$ magnetic phase $T < T_1$, indicating that the nematic order remains critical in the whole temperature range $0 < T < T_{K\text{F}}$. A careful comparison of $\eta_M(T)$ and $\eta_N(T)$ for $T$ below $T_1$ revealed a relation $\eta_N(T) \approx 4\eta_M(T)$, in accord with the expectations of the spin wave analysis.

**Ising transition at $T_1$:** A cartoon picture of the Ising transition is given in Fig. 5 (a), where it is described as the loss of local “head-tail” order. The choice of the order parameter for the transition is not unique and, to the best of our knowledge, has never been given an explicit expression. Here we choose to analyze the temperature dependence of

$$I = (3/L^2) \sum_{i \in \mathcal{A}} \text{sgn}(\cos[\theta_i - \theta_{i0}]),$$

where $\theta_{i0}$ is the spin angle at some reference site $i0$ of the $\mathcal{A}$ sublattice. As an Ising-like variable, $\text{sgn}(\cos[\theta_i - \theta_{i0}])$ carries two allowed values $\pm 1$. In the aN phase, $\theta_i$ and $\theta_i + \pi$ occur with equal probabilities, thus $I = 0$. An excellent data collapse in finite-size scaling was obtained with the 2D Ising critical exponents, $\beta = 1/8$, $\gamma = 1.75$, and $\nu = 1$ for both $x = 0.8$ and $x = 0.9$. To be exact, the orientation of $\theta_i$ with regard to a reference angle $\theta_{i0}$ will be arbitrary as the separation $i - i0$ tends to infinity in a truly thermodynamic system. Given the small exponent $\eta_N(T) < 0.03$ near $T = T_1$ consistent with an extremely slow decay, however, one can argue that the only effective low-energy fluctuation is the $\pi$-flip of the spin (which reverses the sign of $\cos[\theta_i - \theta_{i0}]$).
rather than the small-angle fluctuations (which does not reverse the sign) for the practical system sizes considered in the MC simulation. As far as this is the case, our definition serves as a good measure of the Ising transition.

FIG. 6: Eight possible magnetic patterns within the nematic ordered phase, which also includes configurations with the global rotation of all the spins shown here. The corresponding chirality of each spin configuration is shown inside the triangle.

Chiral-nematic phase: The central finding of this work is the identification of the chiral-nematic phase in the absence of any magnetic order. Although nematic order is algebraically ordered, the chirality, due to its discrete nature, can undergo a true long range ordering.

The case for chiral-nematic order at large $J_2/J_1$ ratio can be made clearly if we consider the $J_1 - J_2$ model with the discrete angles $\theta_i = 2\pi n_i/p$, $p = 6$, and $n_i$ an integer between 1 and 6. The bi-quadratic $J_2$-interaction turns into a 3-state planar model which is known to have a second-order transition (not KT transition) into an ordered phase[19]. In our language, this is the paramagnetic-to-nematic transition. As the small $J_1$ interaction is introduced, the six-fold spin model within the nematically ordered phase is governed by the effective interaction

$$-(J_1/2) \sum_{(ij)} \sigma_i \sigma_j, \quad \sigma_i = \pm 1. \quad (5)$$

where the Ising variable $\sigma_i$ denotes the two opposite orientations of the spin. Due to this residual interaction there will be an Ising phase transition at a temperature $T_1 \approx 3.641 \times (J_1/2) \approx 1.82(1 - x)$ according to known results of the Ising model in two-dimensional triangular lattice. The linear decrease of $T_1$ with $x$ expected from the effective interaction as well as the absolute values of the critical temperatures are consistent with the phase diagram, Fig. 1. Within the nematic-ordered phase, there are eight spin configurations allowed for a triangle as shown in Fig. 6. The chirality for each configuration reads

$$\chi_{ijk} = (\sigma_i \sigma_j + \sigma_j \sigma_k + \sigma_k \sigma_i)/3, \quad \chi \sim \sum (\sigma_i \sigma_j + \sigma_j \sigma_k + \sigma_k \sigma_i) \sim \sum \sigma_i \sigma_j. \quad (7)$$

The final expression, being proportional to the energy, is positive at any temperature $T$ for a ferromagnetic Ising model given in Eq. (5). Therefore the chirality remains non-zero at temperature above $T_1$ where magnetic order is lost, but the nematic order is long-ranged. It is possible that the chirality, due to its discrete nature, can survive the continuum limit $p \to \infty$ and remain long-ranged even as the underlying nematic correlation is algebraically decaying.

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