PHASE TRANSITIONS OF FRUSTRATED
XY SPINS IN TWO DIMENSIONS

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The row model is used to study the commensurate-incommensurate (C-IC) and isotropic (FFTXY) transitions of the frustrated 2D XY model on the triangular lattice. New relevant variables clarify the physics of these transitions: phase and chiral variables are coupled so that spin waves generate long range polar interactions. The resulting dielectric constant diverges at the transition. A single transition occurs for the FFTXY model; in the C-IC regime the Lifshitz point is at $T=0$ and the C phase is a Smectic-A like phase which disorders via a 2D nematic-smectic-A transition.

PACS Numbers 75.10-b, 75.10.Hk

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Frustrated systems have been extensively studied since they constitute non disordered versions of spin-glasses[1][2]. They display rich low-temperature phases and remarkable phase transitions; several non-equivalent wavevectors are found relevant to their physics, reflecting the competing energy scales. As a result, frustration modifies the naive symmetry of the Hamiltonian. For spatial dimensions $D \geq 3$, Kawamura found by renormalization group (RG) techniques that frustrated $O(n)$ spin models belong to a new, “chiral” universality class[3]. He also indicated that commensurability effects studied by Garel and Pfeuty[4] should not play a role near these chiral critical points. For $D = 2$ and XY spins, phase transitions are dominated by defects. Introducing frustration results in additional chiral variables which generate a discrete symmetry. In the fully frustrated case the Hamiltonian for a square lattice is believed to possess an $O(2) \times Z_2$ symmetry[5]; for the triangular lattice (FFTXY) one has the extra $C_{3V}$ symmetry associated with the permutation of the three sublattices, whence adding the possibility of a Potts transition[6]. The transition associated with the $O(2)$ part would be Kosterlitz-Thouless (K-T) -like at a temperature $T_{KT}$ and the discrete $Z_2$ part could be broken below $T_{DS}$. There is an ongoing controversy concerning the order in which these transition should take place. RG calculations and some Monte Carlo (MC) simulations suggest that $T_C = T_{KT} = T_{DS}$ but two transitions are not ruled out[7][8]. In order to unravel the nature of the transition(s) occuring in the fully frustrated case, various schemes have been proposed based on the selective breaking of certain symmetries.

In particular, the row model is a generalization of the FFTXY model where all the bond strengths $J$ are multiplied by $\eta$ in the horizontal direction[9]. The FFTXY model corresponds to $\eta = 1$. In mean field theory, at low temperature and for $\eta < 0.5$ one gets a collinear antiferromagnetic phase (C), whereas for $\eta > 0.5$ an incommensurate spiral (IC) is obtained; a second order (C)-(IC) transition line occurs for $\eta = 0.5$. It extends from $T = 0$ to the Lifshitz point (LP)[10] at $T_L = 1.5J$. A MC algorithm with
“self determined boundary conditions” was developped to study this and other (IC) structures[11] yielding an \( \eta \) versus \( T \) phase diagram quite similar to that predicted in mean field, except that the transition temperature on the (C)-(IC) line depends on \( \eta \). This result was puzzling in view of the fact that the Lifshitz point is at \( T = 0 \) in 2D for the ANNNI model, that the same property holds true for \( O(n) \) spin models with \( n > 2 \) as shown by RG analysis and because of a prediction by Garel and Doniach for the 2D XY model [12].

In this paper we identify a new relevant variable for frustrated systems. Its origin is described below at \( T = 0 \) for simplicity. In standard notations the Hamiltonian of the row model is

\[
\mathcal{H} = - \sum_{<i,j>} J_{ij} \cos(\theta_i - \theta_j)
\]  

(1)

In the ground state, up to a global constant phase \( \theta_i = \vec{Q} \cdot \vec{r}_i \) (\( \vec{Q} \) is the modulation and \( \vec{r}_i \) the position of the ith lattice site). To construct a Villain-type theory[13] for frustrated XY systems we perform local rotations of the axes by an amount \( -\vec{Q} \cdot \vec{r}_i \). In the local frame, all spins are ferromagnetically aligned and their phases \( \phi_i \) are equal to zero. If we excite a spin wave in the local frame (e.g along the \( x \) direction), this distortion modifies the chirality in the laboratory frame and local dipole fluctuations are induced. Spin waves have generated dipolar fields displaying the coupling between phase and chiral degrees of freedom. At low temperature we can estimate the thermal averages of the induced local dipole fluctuation: \( < \delta p > \sim T \sin(\vec{Q} \cdot \vec{r}_{ij}) \) (\( \vec{r}_{ij} \) is the nearest neighbor vector connecting sites i and j); the polarizability \( \alpha \sim 1/T \sum_k < \delta p_i \delta p_k > \sim T \) so that the dielectric constant \( \epsilon_F \sim 1 + o(T/J)[14] \). This T dependence shows that chirality gives the dominant contribution to the total dielectric constant (vortices of the \( \phi_i \) yield \( \epsilon_V \sim 1 + exp - J/T \)). Since the local dipoles are generated in the chiral state the effect vanishes for the (C) case; in the spiral case, since \( \vec{Q} \) does not vary too strongly with \( T \) (see below), \( < \delta p > \) increases with \( T \); the polar energy favors domains parallel to the dipole orientation and opposes the ferromagnetic tendency. When polar forces
overwhelm exchange forces, long range order is lost: this occurs when $\epsilon_F$ diverges in the direction normal to the domains. This process—such that polar effects drive the transitions in the frustrated regime—is a new occurrence of a phase transition determined by the balance between entropy (thermally generated local dipoles) and energy (exchange forces)[15]. For the special case $\eta = 1$ bubble domains are expected to form[16]; owing to the isotropy, vorticies of $\phi_i$ also unbind at the transition. For $\eta$ much less than one, stripe domains are formed when the (anisotropic) dielectric constant diverges in the $x$ direction. This phase, such that the stiffness in the $x$ direction is zero while that in the $y$ direction is finite, is equivalent to the smectic-A phase of liquid crystals. At higher temperature a smectic-A-nematic transition takes place via a K-T melting process[17]: in spin language the stiffness constant in the $y$ direction goes to zero at the paramagnetic boundary. Predictions based on our analytical calculations are in quantitative agreement with MC simulations and support our picture[6][7][18][19].

The starting point of an analysis a-la-Villain[13][20] is to divide excitations into long wavelength and short wavelength contributions. Vortices of the $\phi_i$ and walls of the $\vec{Q}$ will be taken into account for the row model in the defect part of the partition function; as for the long wavelength part we define $\theta_i = \vec{Q} \cdot \vec{r}_i + \phi_i$, where $\vec{Q}$ is for the moment an arbitrary vector, and extend the variations of $\phi_i$ from $-\pi$ to $+\pi$; with this procedure the long wavelength contribution to the partition function of hamiltonian (1) is given by $Z = Tr_{\phi_i} exp - \beta H_{eff}$ where

$$H_{eff} = - \sum_{<i,j>} J_{ij} \cos(\vec{Q} \cdot \vec{r}_{ij}) \cos(\phi_i - \phi_j) - T \log[\cosh(\sum_{<i,j>} \beta J_{ij} \sin(\vec{Q} \cdot \vec{r}_{ij}) \sin(\phi_i - \phi_j))]$$

(2)

The first term is the contribution of the phase variables and the second term is the new relevant (chiral) polar contribution. The Villain form is obtained from (2) by seeking the best hamiltonian quadratic in $\phi_i - \phi_j$: $H_0 = \sum_{<i,j>} \tilde{J}_{ij} (\phi_i - \phi_j)^2$ [21]. The corresponding free energy $F$ is a function of the parameters $\vec{Q}$ and $\tilde{J}_{ij}$. All
computational details are to appear in a forthcoming publication[19]. The effect of the second term of (2) is seen on Figure 1 which shows $\tilde{J}_{ij}$ as a function of distance and also its sign, for various $\eta$. As advertized it is a long range interaction and for large values of $r_{ij}$, $\tilde{J}_{ij} \sim 1/r_{ij}^6$; this feature causes the stiffness of the $\phi_i$ – given by $\gamma \tilde{e} = \sum_j \tilde{J}_{ij}(\vec{r}_{ij} \cdot \vec{e})^2$ in a direction denoted by $\vec{e}$ – to be dramatically depressed.

This is most easily seen for the special case $\eta = 1$ where, had we neglected the (chiral) polar contribution of (2), we would have found the incorrect low temperature result $\gamma = \gamma_0(1 - T/3J)$. Including the long range effects yields $\gamma = \gamma_0(1 - T/J[17/24 - 21/(16\pi\sqrt{3})])$, in excellent agreement with MC data and with Minnhausen’s prediction[6][11][18]. As expected, the difference between the incorrect result and the correct one is due to $\epsilon_F$ which contributes to order $T$. At $T_c \simeq 0.51J$ – a value which agrees well with MC estimates except Ref.8 – both $\gamma$ and $\partial^2 F/\partial Q^2$ vanish; since $\partial^2 F/\partial Q^2$ is proportional to the inverse dielectric constant of the system averaged over the spin wave ensemble (an important feature which we emphasize below), the dielectric constant diverges at $T_c$ and vortex excitations of $\phi$ and defects of $\vec{Q}$ occur. Figure 2a shows the stiffness as a function of temperature; on the same plot we have represented the points obtained by performing a MC simulation of the FFTXY. The agreement extends all the way into the critical region. We attribute this property to the fact that $Q$ remains pinned to its $T = 0$ value so that large phase fluctuations do not occur except right at $T_c$. The value of $T_c$ that comes out of our equations could have been obtained by equating a dipolar energy to the bond energy: $\pi \tilde{J}sin(\vec{Q} \cdot \vec{r}_{ij})^2(T/3\tilde{J})^2 \sim \tilde{J}$. At $T_c$ the specific heat diverges; the scaling will be presented elsewhere[19].

We now turn to the case when a (IC)-(C) transition may occur. Figure 2b shows the stiffnesses in the x and y directions. We notice that $\gamma_x$ goes to zero at some temperature but the corresponding $\gamma_y$ remains finite. As one approaches the boundary where the dielectric constant diverges in the x direction, fluctuations in
$Q_x$ become large. Thus our curve is not as close to the MC data near $T_c \approx 0.22J$ as before[11][19]. On the other hand the wavevector remains commensurate in the $y$ direction at all temperature. We show $Q_x(T)$ in the inset of Figure 2b; note that it does not go to $\pi$ at the transition. As explained in the introduction, the homogeneous state is unstable because of polar effects. This has two important implications. First, the dipolar fluctuation, which is proportional to $\sin(\vec{Q} \cdot \vec{r}_{ij})$ does not vanish and is always a relevant variable at higher temperature; this is why polar forces dominate. Second, we see that because $Q_x = \pi$ is not an allowed solution, there is no incommensurate-commensurate boundary except at $T = 0$. Increasing the temperature beyond $T_c$, the stiffness is zero in the $x$ direction and non zero in the $y$ direction. Along $x$, polar interactions have broken the samples into stripes parallel to $y$[22-25]; MC simulations in fact do show that behavior, seen in Figure 3. The local $Q_x$ is pinned to its $T_c$ value, but globally there is no rigidity along $x$. We can describe this situation within our formalism by incorporating a spatial dependence to $Q_x$. The theory then resembles that of the dipolar magnet. The above characteristics can be summarized by writing the long wavelength free energy

$$F(\phi) = \int d^2 r [\lambda (\partial_x \phi)^4 + \gamma_y (\partial_y \phi)^2]$$

This is a de Gennes-like free energy of a Smectic-A liquid crystal[17]. The lack of spin order along $x$ corresponds to the absence of translational order in the layers. The layering of the smectic is the spin order in the $y$ direction. As shown by Day et al.[17], the smectic phase turns into a nematic phase above a K-T melting temperature. In our case the transition between the “smectic-like” phase and the paramagnetic phase is in the same universality class as the liquid crystal case. This implies that for fixed $\eta$, as one varies the temperature, one goes from the (IC) phase to the “smectic-like” phase to the paramagnetic phase. The only place where the (IC) and (C) phases meet is at $T = 0$. Thus, for the row model the Lifshitz point is at $T = 0$ for 2D XY systems[12].

We now discuss the physical content of hamiltonian (2). We may apply
the scheme that we described to a situation where no frustration is present, e.g. for purely ferromagnetic interactions. In that case the preferred thermodynamic $Q$ is zero, the $\tilde{J}_{ij}$ are short range, and we are simply computing the effect of spin waves in a ferromagnet. However, as stressed above, $\partial^2 F / \partial Q^2$ is proportional to the inverse dielectric constant averaged over the spin wave hamiltonian and is always less than $\gamma$. Since in the low temperature phase of the XY model the renormalized theory is a spin wave theory $\partial^2 F / \partial Q^2$ gives a fair estimate of the true value of the dielectric constant except close to $T_c$ where vortices contribute significantly. Applying the K-T criterion with $\partial^2 F / \partial Q^2$ gives a determination of $T_c^{SW}$ that differs from the MC $T_c$ by 14% (for the square lattice we get $T_c \approx 1.02J$ and for the triangular lattice $T_c \approx 1.66J$, compared to the MC values of 0.89J and 1.45J respectively[26]); the vortex contribution to the dielectric constant accounts quantitatively for the difference[14]. Yet the spin wave hamiltonian misses the transition since neither $\gamma$ nor $\partial^2 F / \partial Q^2$ vanishes at $T_c^{SW}$, unlike the frustrated case. The reason for the above properties is that we have constructed a canonical ensemble where the macroscopic phase is free to adjust thermodynamically, as opposed to the microcanonical procedure of fixing the phase a priori. In that latter ensemble it is necessary to introduce a twist of the phase across the sample or to modify the boundary conditions to extract the stiffness constants. In the canonical ensemble these quantities appear naturally. The fluctuations of $\vec{Q}$ affect both the frustrated and unfrustrated systems. In the frustrated case these fluctuations are crucial to determine the phase transitions. Even from the standpoint of MC simulations one sees that ”self-determined” boundary conditions are likely to produce a more effective thermal equilibration. This is indeed what we have noticed in our MC simulations.

To conclude, we have constructed an appropriate Villain-like theory to describe phase transitions of modulated systems and of the fully frustrated XY model in 2D. This is achieved by performing local rotations which align the spins ferromag-
netically in the ground state. The long wavelength fluctuations consist of spin waves coupled to dipolar fields. These fields weaken the order by generating an effective dielectric constant which diverges at $T_c$. Our results show that in the isotropic limit (FFTXY) a single transition occurs. In the modulated case a transition is seen between a spiral phase and a smectic-A type of order consisting of stripes of correlated spins in one direction but without long range order in the other direction. At higher temperature a smectic-A-nematic transition to the paramagnetic phase is expected; the Lifshitz point is thus at $T = 0$ in accord with Garel and Doniach. In our approach the local rotations are also thermal variables. They define the macroscopic phase of the system in the ordered state which is – in our derivation – a true thermodynamic quantity. Our method is quite general and applies to many physical situations where phase fluctuations are relevant.

**Acknowledgments** We enjoyed fruitful discussions on this problem with T. Garel who provided us with a helpful clue on the smectic-A-nematic transition. Support from NATO grant CRG 930988 and from IDRIS for computer time on the Cray C98 contrat 940162 are gratefully acknowledged.
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FIGURE CAPTIONS

FIG. 1.

\[ \ln(\tilde{J}_{ij}) \text{ vs } \ln(r_{ij}) \text{ for } T=0.1J; \text{ solid line } \eta = 1, \text{ dashed line } \eta = 0.575. \]
 Insets: sign of \( \tilde{J}_{ij} \) at position \( \vec{r}_{ij} \); negative values are denoted by circles; upper inset \( \eta = 1 \), lower inset \( \eta = 0.575 \).

FIG. 2.

(a) \( \partial^2 \mathcal{F}/\partial Q^2 \text{ vs } T/J \) for \( \eta = 1 \) (solid line). Crosses: results of a MC simulation for a 30x30 FFTXY. (b) Stiffnesses along x (solid line and left scale) and along y (dashed line and right scale) versus T/J for \( \eta = 0.575 \). Crosses: results of a 30x30 MC simulation. Inset \( Q_x(T) \text{ vs } T/J \).

FIG. 3.

Stripe structure for \( \eta = 0.575, T = 0.4 \) : MC simulation of a 36x36 triangular lattice. Closed, open circles and empties denote plaquettes of positive, negative and zero chirality respectively.