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Dynamics of spin and chiral ordering in the two-dimensional fully frustrated XY model

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We present simulation results on the ordering dynamics of the fully frustrated XY model (FFXYM) in a two-dimensional square lattice which possesses $O(2)\times Z_2$ symmetry, using the Langevin dynamics approach with initial disordered state quenched to low temperature. The spin correlation functions satisfy a critical dynamic scaling of the form $C_S(r,t)=r^{-\eta(T)}g_S(r/L_S(t))$ where $\eta(T)$ is the critical exponent for the equilibrium spin correlation function at temperature T and $L_S(t)\sim t^{1/z_S(T)}$. Ising correlation due to the extra Z_2 symmetry shows a dynamic scaling behavior $C_I(r,t)=g_I(r/L_I(t))$ with $L_I(t)\sim t^{1/z_I(T)}$. Both dynamic exponents $1/z_S$ and $1/z_I$ are strongly *temperature-dependent* increasing in proportion to T at low temperature. Simulation shows that there exist two regimes with distinct domain growth morphology. A qualitative explanation of these features is given in terms of the interplay between thermal fluctuations and the long range nature of the interaction between point defects.

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When statistical systems are quenched from a disordered phase to an ordered phase, they evolve into an ordered phase via the growth of ordering regions. The average size of ordered domains grows with time and becomes the dominant length scale at the late stage of the ordering processes which leads to a simple dynamic scaling in the order parameter correlation functions. Predicting how the average domain size grows with time and computing the scaling functions from first principles are a few fundamental issues in this area [1]. Recent interest in this field is mainly concentrated on systems with continuous symmetry [2–4]. For these systems, the continuous nature of order parameter space allows rich stable topological defects such as vortices, strings, and monopoles which are shown to play crucial roles as disordering agents in the coarsening processes [5].

Now, if a system has *both* discrete *and* continuous degeneracies in its ground states, one can anticipate that its ordering dynamics may be richer and more interesting. Here, we investigate the ordering dynamics of the fully frustrated XY model (FFXYM) in a two-dimensional square lattice. In equilibrium, this model can be realized physically as two-dimensional arrays of Josephson junctions under magnetic fields of half flux quantum ($f=\frac{1}{2}$) per unit plaquette. It is well known that the pure XY model undergoes a Kosterlitz-Thouless (KT) transition at the temperature T_{KT} due to the unbinding of bound vortex pairs [6]. For FFXYM the system possesses additional discrete Ising-like Z_2 symmetry corresponding to the double degeneracy of the chirality configuration as well as continuous O(2) symmetry corresponding to the global uniform phase rotation, leading to the new Ising-like phase transition at the temperature T_I. Numerically, T_{KT} and T_I for FFXYM are very close to each other ($T_{KT}\approx T_I\approx 0.45J/k_B$), even though there are still controversies as to whether the two transitions occur at exactly the same temperature or at close but distinct temperatures [7].

Hence, in this system, the line defects associated with the discrete Ising symmetry coexist with the point defects (which turn out to be the corners of the line defects) associated with the continuous O(2) symmetry and the interaction between these defects play an important role in the ordering processes [8]. We focus mainly on the temperature dependence of scaling exponents associated with the growth of the two kinds of order parameters by quenching the system to various final temperatures below both T_{KT} and T_I. Simulations show that spin correlations satisfy critical dynamic scaling, while the Ising correlation follows simple dymamic scaling. Growth exponents for both correlation functions are strongly *temperature dependent* with linearly proportional dependence in T at very low temperature. In the limit of zero temperature, the growth process becomes indefinitely slow and zero temperature freezing is observed. Another interesting feature of the growth dynamics of this system is that there exist two temperature regimes with qualitatively different characteristics of domain growth, especially that of morphology of Ising domain walls which is manifested in the relaxation scaling behavior of various quantities. For quench to a low temperature below $T_R\simeq 0.3J/k_B$, we observe the faceted growth of domain walls where line defects are mostly straight with a relatively few number of corners (point defects). On the other hand, for quench to an intermediate temperature above T_R (and of course below T_I and T_{KT}), we observe microscopically *rough* line defects with a dense distribution of corners. We attribute these features to the interplay between thermal fluctuations and the long range nature of the interaction between point defects that gives rise to a chemical potential for creating a pair of corners.

The system is defined by the following Hamiltonian:

$$H=-J\sum_{\langle ij\rangle}\cos(\theta_i-\theta_j-2\pi f_{ij}), \tag{1}$$

where θ_i is the phase angle of the planar spin $\vec{S}_i$ at site i and $\langle ij\rangle$ denotes the summation over nearest neighbors. The frustration of the model is determined by f_{ij} with $f\equiv\Sigma_{(ij)\in P}f_{ij}=\frac{1}{2}$ where P denotes a unit plaquette. The dynamics is assumed to be purely dissipative (with nonconserved order parameter) and governed by the following Langevin equation:

$$\partial\theta_i/\partial t=-\Gamma([\delta H(\{\theta_k,f\})]/\delta\theta_i)+\zeta_i(t), \tag{2}$$

where Γ is the kinetic coefficient and the thermal noise $\zeta_i(t)$ is chosen to be a white Gaussian with zero mean and with the variance satisfying the detailed balance at temperature T,

$$\langle\zeta_i(t)\zeta_j(t')\rangle=2\Gamma k_BT\delta_{ij}\delta(t-t'). \tag{3}$$

Equation (2) together with Eq. (3) is integrated in a straightforward way by using the Euler method with periodic boundary condition. Most simulations were performed on lattices of size $N_x\times N_y=128\times128$ with the integration time step $\Delta t=0.05$ and the results were averaged over 30 different random initial configurations.

The main quantities of interest are spin correlation and chiral correlation functions. The so-called *zero momentum* gauge-invariant spin correlation is defined as follows:

$$C_S(r,t)=\left\langle\frac{1}{N_xN_y}\sum_i\cos\left(\theta_{i+r}-\theta_i+2\pi\sum_{(kk')\in\gamma}f_{kk'}\right)\right\rangle, \tag{4}$$

where $\langle\ \rangle$ denotes the average over random initial configurations and γ represents the path along which the correlation function is calculated. For convenience, we evaluated the spin correlation for only even lattice spacing along the x and y axes (the gauge term drops out in this case) and took the average over the two results. The *staggered* chirality for a plaquette P_R with the Cartesian coordinate of its center at $R=(R_x,R_y)$ is defined as

$$\chi(R)=(-1)^{x+y}\mathrm{sgn}\left[\sum_{P_R}(\theta_i-\theta_j+2\pi f_{ij})-2\pi f_{\mathrm{nint}}[(\theta_i-\theta_j+2\pi f_{ij})/2\pi]\right], \tag{5}$$

where f_{nint} is the nearest integer function and the dual lattice vector is $R=(R_x,R_y)=[(x+1/2)a_0,(y+1/2)a_0]$ with a_0 the lattice spacing which will be taken to be 1 from now on. The chiral (Ising) correlation function is defined as

$$C_I(r,t)=\left\langle\frac{1}{N_xN_y}\sum_i\chi_{i+r}\chi_i\right\rangle. \tag{6}$$

Due to the existence of these two kinds of order parameters the relaxation and ordering process proceeds via annihilation of two kinds of defects, i.e., point defects [corresponding to O(2) symmetry] and line defects (domain walls corresponding to chiral symmetry). Point defects are the corners of line defects where fractional charges of magnitude $\frac{1}{4}$ reside [9]. Hence, the annihilation processes of these two kinds of defects are closely coupled to each other. At finite temperatures below T_{KT} and T_I ($T_{KT}\approx T_I\approx0.45J/k_B$), the ordering dynamics shows an interesting temperature dependence. Spin correlation satisfies (similarly to the case of the pure XY model) a critical dynamic scaling [10]

$$C_S(r,t)=r^{-\eta(T)}g_S(r/L_S(t)), \tag{7}$$

where $\eta(T)$ is the critical exponent for the equilibrium spin correlation function at temperature T and $L_S(t)\sim t^{1/z_S}$, while the chiral correlation obeys the following usual scaling form

$$C_I(r,t)=g_I(r/L_I(t)) \tag{8}$$

with $L_I(t)\sim t^{1/z_I}$. Though there is no analytic result known for the temperature dependence of the critical exponents $\eta(T)$, $z_S(T)$, and $z_I(T)$ for FFXYM, in contrast to the case of the pure XY model, our estimates for the exponent $\eta(T)$ are a little larger than the values obtained from the recent extensive (equilibrium) Monte Carlo simulations carried out by Ramirez-Santiago and Jose [11]. Regarding the dynamic exponents, to our knowledge, our results provide the only numerical estimates for their temperature dependence. We also find it interesting that the short distance behavior of the chiral scaling function $g_I(x)$ satisfies the generalized Porod's law [3,4,12] $g_I(x)=1-a(T)x^{\phi(T)}$, where $a(T)$ is the temperature dependent amplitude and the exponent $\phi(T)$ decreases continuously starting from Ising value 1 near zero temperature as the final quenching temperature becomes higher [13].

Figures 1(a) and 1(b) show the scaling collapse of spin correlation, and chiral correlation, respectively, at $k_BT=0.2J$. The inset of Fig. 1(a) shows the temperature dependence of η that exhibits an approximately linear increase in T at low temperature. As mentioned earlier, these values obtained from the dynamic scaling collapse are a little bigger than the equilibrium Monte Carlo results (on a smaller lattice size) and more detailed simulation is needed to resolve the discrepancies. Note that the exponents $1/z_S$ and $1/z_I$ are appreciably smaller than 0.5 at $k_BT=0.2J$. Our simulations show that, in contrast to the case of the pure XY model, these exponents ($1/z_S$ and $1/z_I$) depend strongly on temperature especially at the low temperature regime which is shown in the inset of Fig. 1(b). We can see that these two exponents increase approximately linearly in T at low temperatures and then they saturate at around $k_BT\sim0.35J$ with saturation values of around 0.45 for $1/z_S$ and 0.5 for $1/z_I$. In addition, we find that the two exponents are quite close to each other for the low temperature regimes. However, $1/z_I$ tends to be slightly larger than $1/z_S$ as the temperature gets larger than $k_BT\simeq0.2J$.

In order to help our understanding of these temperature-dependent dynamic exponents, we looked into the snapshots at various time instants of ordering configurations in terms of staggered chirality. Figures 2(a) and 2(b) show the ordering processes for a quench to low temperature and higher temperature ($k_BT=0.1J$ and $k_BT=0.4J$, respectively), where domains with opposite Ising order parameter (staggerred chirality value) are denoted with different shades. We can clearly see a distinctive feature in the domain growth morphology for the low and high temperature systems. That is, at low temperature, the domain walls (line defects) become more and more straight in time with faceted (square shaped) boundaries, while at higher temperature the domain walls remain rough microscopically all along the ordering process. Slow ordering for the case of low temperature ($k_BT=0.1J$) relative to that of high temperature ($k_BT=0.4J$) is apparent

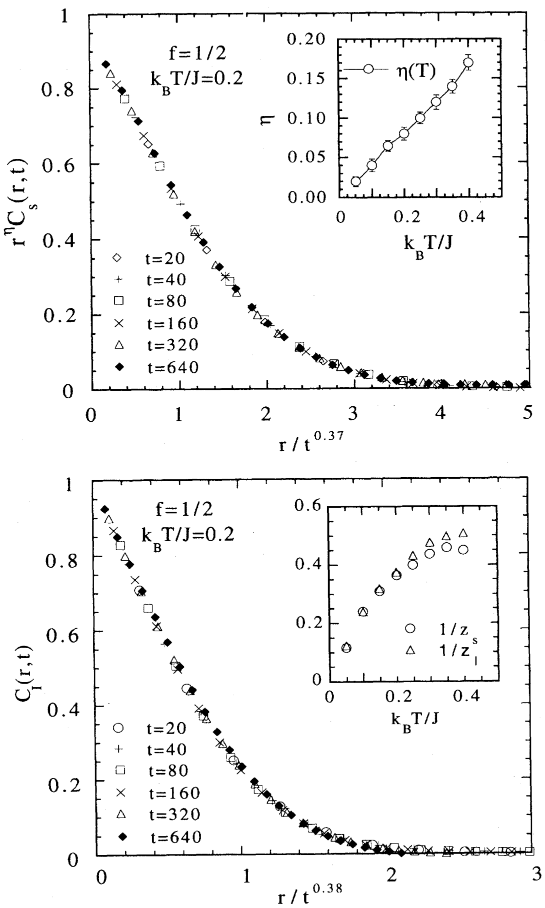

FIG. 1. Scaling collapse of spin correlation (a) and chiral correlation (b) at $k_BT=0.2J$ for FFXYM with lattice size 128×128, which gives $1/z_S \simeq 0.37$, $\eta(k_BT=0.2J)\simeq 0.08$, and $1/z_I \simeq 0.38$. The inset of (a) shows the temperature dependence of $\eta(T)$ obtained from critical dynamic scaling and the inset of (b) shows the temperature dependence of $1/z_S$ and $1/z_I$. Error bars for quantities in the inset of (b) are a few times the size of the symbols.

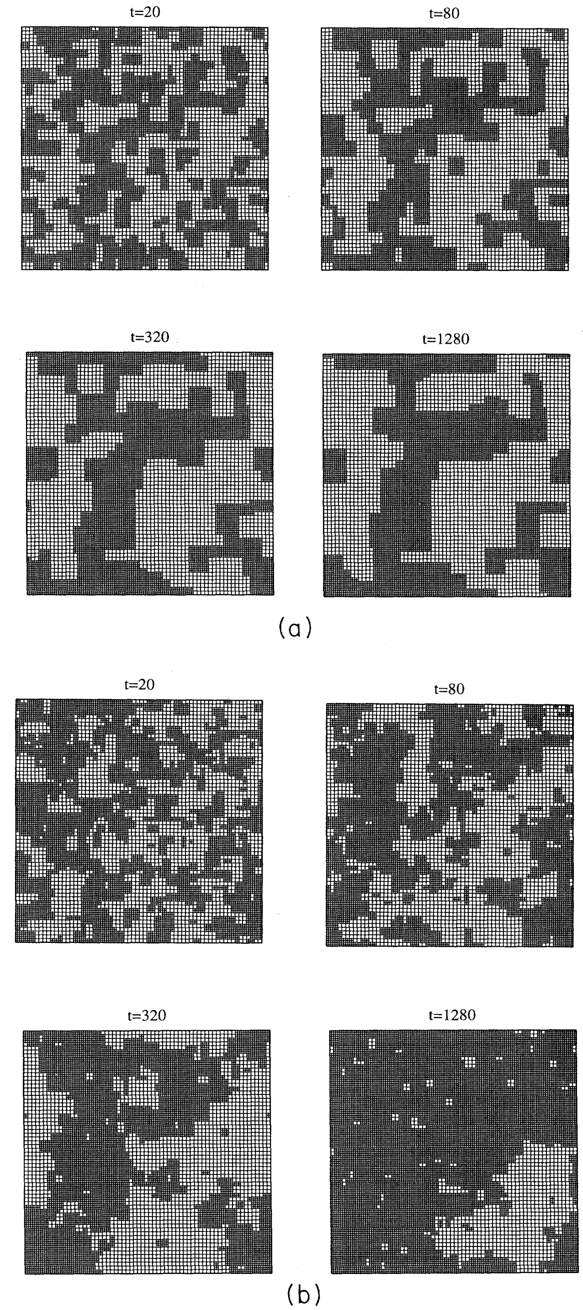

FIG. 2. Snapshots at various time instants of Ising (staggered chirality) domain configuration at $k_BT=0.1J$ (a) and at $k_BT=0.4J$ (b). Slow growth of ordering is apparent in the case of $k_BT=0.1J$ compared with that of $k_BT=0.4J$. Note the different domain morphology in the two cases with faceted domain walls in the case of $k_BT=0.1J$ and rough domain walls in the case of $k_BT=0.4J$.

from these figures in agreement with the temperature dependence of $1/z_I$ obtained from scaling collapse of chiral correlation functions.

In relation to the above morphological features, it would be interesting to calculate the time dependence of the number of point defects ($\equiv N_p$) and that of the total length of the line defects ($\equiv N_l$) and compare the results with other exponents already presented. We found from simulations that they show power law decay behavior in time with temperature-dependent exponents. That is, we get $N_p \sim t^{-\nu_p}$ and $N_l \sim t^{-\nu_l}$. These exponents together with $1/z_S$ and $1/z_I$ are shown in Fig. 3 as functions of the temperature. We can recognize that there exists a temperature scale ($\simeq T_R$) which roughly divides the temperature regime into two subregimes with different scaling behavior. We see that $k_BT_R \simeq 0.3J$. Below T_R (regime I), we have $\nu_p > \nu_l$ which means that point defects decay away faster than the line defects resulting in straight domain walls with occasional corners (point defects) and faceted growth of the domain walls. This expectation is in qualitative agreement with Fig. 2. Above T_R (regime II), on the other hand, we have $\nu_p \simeq \nu_l$, which can be interpreted as corresponding to microscopically rough domain walls with the average distance between neighboring point defects (corners) along a line defect being kept constant in time, as is also seen in Fig. 2.

In dual pictures, in terms of point and line defects, we

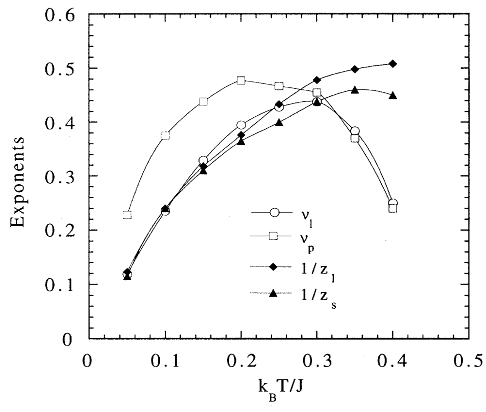

FIG. 3. The temperature dependence of various exponents ($1/z_S$, $1/z_I$, ν_l, ν_p). Error bars are a few times the size of the symbols. See the text for details.

may be able to understand qualitatively the slow growth process and small values of $1/z_S$ and $1/z_I$ at the lower temperature regime (regime I) if we consider the fact that the total energy of the system not only comes from the total length of the line defects but also from the long range Coulomb interaction between point defects, namely the corners of the line defects. This means that the system has to pay some amount of energy (chemical potential) in order to create a pair of local point defects even without increasing the length of the domain wall. Therefore at zero temperature an isolated domain wall in the shape of a large rectangle cannot change its shape due to the energy barrier for local change of its shape (hence they are *pinned* metastable configurations). This would explain the zero temperature freezing in the growth process [14]. At finite but still very low temperature, only occasional decays of the above-mentioned rectangular shapes would occur through the thermal activation process and we expect that the growth would proceed slowly with the growth exponents increasing as the temperature increases. At higher temperature (regime II), the barrier energy would now be easy to overcome (hence rough domain walls), but on the other hand thermal fluctuations will partly hinder the ordering processes, which leads to saturated values of the growth exponents in regime II.

In summary, we presented simulation results on the ordering kinetics of fully frustrated *XY* models in a two-dimensional square lattice focusing on the effect of the interaction between discrete and continuous symmetry and corresponding defects on the relaxation and (quasi-) ordering processes. A more detailed analysis, including staggered chirality and the autocorrelation functions, will be presented elsewhere [13]. It would be interesting to investigate the related but more general case of systems with coupled order parameters such as $Z_2\times O(N)$ symmetry in arbitrary dimensions. It would also be of some interest to study the ordering dynamics of the Ginzburg-Landau model corresponding to FFXYM in order to see whether that model retains the same characteristics of domain growth as FFXYM as presented in this work.

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[1] J. D. Gunton *et al.*, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1983) Vol 8; H. Furukawa, Adv. Phys. **34**, 703 (1985); K. Binder, Rep. Prog. Theor. Phys. **50**, 783 (1987).

[2] G. F. Mazenko and M. Zannetti, Phys. Rev. Lett. **53**, 2106 (1984); Phys. Rev. B **32**, 4565 (1985).

[3] A. J. Bray and S. Puri, Phys. Rev. Lett. **67**, 2670 (1991).

[4] F. Liu and G. F. Mazenko, Phys. Rev. B **45**, 6989 (1992) and references therein.

[5] A. J. Bray, in *Phase Transitions in Systems with Competing Energy Scales*, edited by T. Riste and D. Sherrington (Kluwer Academic, Boston, 1993).

[6] J. M. Kosterlitz and D. Thouless, J. Phys. C **6**, 1181 (1973); J. M. Kosterlitz, *ibid.* **7**, 1046 (1974).

[7] S. Teitel and C. Jayaprakash, Phys. Rev. B **27**, 598 (1983); W. Shih and D. Stroud, *ibid.* **28**, 6575 (1983); M. Y. Choi and S. Doniach, *ibid.* **31**, 4516 (1985); T. Halsey, J. Phys. C **18**, 2437 (1985); M. Yosefin and E. Domany, Phys. Rev. B **32**, 1778 (1985); G. S. Grest, *ibid.* **39**, 9267 (1989); J. Lee *et al.*, *ibid.* **43**, 11 531 (1991); D. B. Nicolaides, J. Phys. A **24**, L231 (1991); G. Ramirez-Santiago and J. V. Jose, Phys. Rev. Lett. **68**, 1224 (1992); J. R. Lee, Phys. Rev. B **49**, 3317 (1994); S. Lee and K. C. Lee, *ibid.* **49**, 15 184 (1994).

[8] Rigorously speaking, at *finite T*, the spin order parameter [corresponding to O(2) symmetry] attains only quasi-long-range order at equilibrium with power law correlation of continuously varying exponents (critical line). Therefore, in that case, the approach to equilibrium critical state may be termed a "*quasi-ordering* process."

[9] T. C. Halsey, J. Phys. C **18**, 2437 (1985).

[10] Jong-Rim Lee *et al.* (unpublished).

[11] G. Ramirez-Santiago and J. V. Jose, Phys. Rev. B **37**, 9567 (1994).

[12] G. Porod, in *Small Angle X-Ray Scattering*, edited by O. Glatter and L. Kratky (Academic, New York, 1983).

[13] Sung Jong Lee *et al.* (unpublished).

[14] Z. W. Lai *et al.*, Phys. Rev. B **37**, 9481 (1988).