Kinetics of phase ordering in the two-dimensional coupled XY-Ising model

Jong-Rim Lee,[1] Sung Jong Lee,[2] Bongsoo Kim,[3] and Iksoo Chang[1]
[1] *Department of Physics, Pusan National University, Pusan, 609-735, Korea*
[2] *Department of Physics, The University of Suwon, Hwasung-Gun, Kyunggi-Do, 445-890, Korea*
[3] *Department of Physics, Changwon National University, Changwon, 641-773, Korea*

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The ordering kinetics of a coupled XY-Ising model on a two-dimensional square lattice quenched from a disordered state to a low-temperature ordered phase is investigated via Monte Carlo dynamical simulations. The decay process of the two types of topological defects (point vortices and line defects of Ising domain walls) and the interaction between them controls the long-time dynamics of the ordering. In particular, the decoupling of XY degrees of freedom across Ising domain walls leads to the pinning of vortices near the walls, which considerably slows down the growth of XY order: it shows a power-law growth in time with the exponent $\phi_{XY}\simeq 0.38$. This vortex pinning also appears to give rise to a stretched exponential relaxation in the XY autocorrelation function. The dynamic scaling for both XY and Ising order parameters in the presence of multiple length scales is discussed. [S1063-651X(96)09609-2]

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I. INTRODUCTION

Understanding the ordering kinetics of statistical systems subjected to a rapid thermal quench from a disordered phase to an ordered phase has been one of the central issues in non-equilibrium statistical mechanics [1,2]. A recent nonperturbative approach to this problem [3–5] seems to offer significant theoretical progress in this area. Being extended to systems possessing continuous degeneracy of ground states, the theory [6–8] has stimulated intensive theoretical and experimental investigations on the kinetics of systems having a variety of stable topological defects such as vortices, strings, and monopoles.

Most research so far, however, have been restricted to systems with ground states possessing a *single* type of degeneracy, either discrete or continuous. Recently, Lee, Lee, and Kim [9] have investigated numerically the kinetics of ordering in a system with both discrete and continuous symmetries. This work indicated that the ordering kinetics of systems having *two* types of ground-state degeneracies simultaneously can be, though complicated, very rich due to the simultaneous presence of two different stable topological defects and the interaction between them. Specifically, the model they considered was the two-dimensional fully frustrated XY model (FFXYM) [10] on a square lattice. The ground-state manifold of the model possesses discrete Ising-like chiral symmetry in addition to usual global continuous rotation symmetry in spin space. Due to this unusual symmetry structure of the ground-state manifold, excitations of the model can have two types of stable topological defects: line defects of chiral domain walls and point defects, which are vortices having a fractional value of the original vortex charges and reside always at the corners of the line defects [11,12]. Simulation showed that the interaction between two kinds of defects leads to an unusual faceted domain morphology at low temperatures, which becomes rough at some finite temperature.

A coupled XY-Ising model [13], which explicitly has both XY and Ising degrees of freedom on each site, is another model system having the same $O(2)\times Z_2$ ground-state degeneracies as the FFXYM. Here the O(2) continuous symmetry corresponds to the invariance of Hamiltonian under global rotation of phases of XY spins, whereas the Z_2 discrete symmetry corresponds to the doubly degenerate Ising order parameter. This model, with an appropriate choice of the parameters, has been claimed to belong to the same universality class as the FFXYM with respect to the equilibrium critical properties. In the present work, we carry out Monte Carlo simulations on the ordering kinetics of a coupled XY-Ising model with the aim of highlighting the common and contrasting features of these two closely related models possessing the same ground-state degeneracies.

We find that the Monte Carlo ordering kinetics of the coupled XY-Ising model in two dimensions exhibits interesting features due to the mutual pinning between point vortices and Ising domain walls. In the limit of a zero-temperature quench, the system freezes into metastable configurations, just as in the case of pure hard spin XY model [14,15] or the FFXYM in two-dimensional square lattices [9]. For quenches to finite temperatures, the equal-time correlation functions of an Ising order parameter satisfy a dynamic scaling, while those of an XY order parameter follow a critical dynamic scaling, as can be expected from the fact that the XY order parameter, at equilibrium, exhibits a so-called Kosterlitz-Thouless (KT) phase [16] with a power-law correlation for $T<T_{\mathrm{KT}}$, where T_{KT} is the KT transition temperature. The appropriate length scales (corresponding to the average size of Ising domain L_I and the XY-ordered region L_{XY}) exhibits power-law growth in time, i.e., $L_I\sim t^{\phi_I}$ and $L_{XY}\sim t^{\phi_{XY}}$ with temperature-dependent growth exponents ϕ_I and ϕ_{XY}: they show a quick increase at low temperature and saturate to the values near $\phi_I\simeq 0.5$ and $\phi_{XY}\simeq 0.38$, respectively, for most of the temperature range below the transition temperature $T_I\sim T_{XY}\simeq 1.38$. The simulation result that the growth exponent ϕ_{XY} for the XY quasiordering is significantly smaller than that of the pure XY model [17–19,15] can be attributed to the effect of pinning the vortices near

Ising domain walls, which hinders the motion of point vortices and also the annihilation of vortex-antivortex pairs.

In terms of the domain growth morphology, we find that, at low temperatures, Ising domain walls show mostly faceted shapes (straight domain walls), while at higher temperature they become rough. This fact is in contrast to the case of pure Ising dynamics where the infinitesimal thermal fluctuation leads to rough domain walls. In the case of the FFXYM, quite convincing numerical evidence [9] could be given to the finite-temperature roughening of the chiral domain walls, which was attributed to the interplay between the long-range interaction of corner point defects (with fractional charges) and the thermal fluctuation. In the case of a coupled XY-Ising model, the status of numerical evidence as to the finite-temperature roughening is not conclusive enough. There are no inherent charges associated with corners of Ising domain walls in the coupled XY-Ising model. But the decoupling of XY spins across Ising domain walls (see below) makes the vortices of XY spins pinned near Ising domain walls or corners, which may play roles similar to the corner charges in the FFXYM.

We find a feature for the autocorrelation function of the XY spin order parameter that exhibits an unusual stretched exponential behavior of $A_{XY}(t) \sim \exp(-ct^{\beta})$, where the value of β ranges from 0.13 to 0.17. This peculiar behavior is reminiscent of the behavior of the spin autocorrelation in the one-dimensional XY model, but with a different value of the exponent β ($\beta = 1/2$ in the one-dimensional XY model) [20]. A similar stretched exponential behavior for the XY autocorrelation function is found in a time dependent Ginzburg-Landau model with both XY and Ising-type ground-state degeneracies where the value β is given approximately by $\beta \simeq 0.16$ [21].

This paper is organized as follows. Section II describes the model, the simulation method, and the quantities of interest. The simulation results along with a discussion are presented in Sec. III. Section IV summarizes the results.

II. MODEL AND SIMULATION METHOD

A general form of the Hamiltonian for a coupled XY-Ising model [13] can be written as

$$\mathcal{H} = -J\sum_{\langle ij \rangle} [(1+\alpha s_i s_j)\cos(\theta_i - \theta_j) + \gamma s_i s_j], \qquad (1)$$

where $s_i = \pm 1$ and θ_i are the Ising spin and the phase angle of the XY spin at site i respectively, and the bracket $\langle ij \rangle$ indicates that the sum is taken over nearest-neighbor pairs. In equilibrium, the model is known to have a rich variety of critical behaviors. For example, Granato *et al.* [13] predict for $\alpha = 1$ (isotropic case) a single continuous transition to a disordered phase (for $\gamma \leqslant \gamma^*$, where $\gamma^* \approx 0.3$) where both XY and Ising orders are destroyed, a separate XY and Ising transition (for $\gamma > \gamma^*$), and a first-order transition (for $\gamma \leqslant \gamma^*$).

In the present work, however, we restrict ourselves to the simplest case of the general Hamiltonian (1), namely, $\alpha = 1$ and $\gamma = 0$:

$$\mathcal{H} = -J\sum_{\langle ij \rangle} [(1+s_i s_j)\cos(\theta_i - \theta_j)]. \qquad (2)$$

Granato *et al.* claim that this simpler model has *single XY* and Ising transition at the temperature $T_c \simeq 1.38$ [22] (we set $J = 1$ and the Boltzmann constant $k_B = 1$). In equilibrium, this model can have two topological excitations at finite temperatures besides the smooth spin wave excitation of the XY spins. One is vortices of the XY spins that interact logarithmically in the large distances among themselves. The other is the domain wall excitation that comes from the two degenerate Ising spin domains. The form of the Hamiltonian (2) indicates that the XY spins located across Ising domain walls (at sites i and j) become decoupled since $1 + s_i s_j = 0$.

We are interested in understanding the kinetics of the ordering process in the system governed by the Hamiltonian (2) followed by a thermal quench from a disordered phase to an ordered phase. The ordering kinetics is probed via Monte Carlo simulations where the standard Metropolis update is carried out from disordered random initial configurations. One of the following update procedures are randomly se-

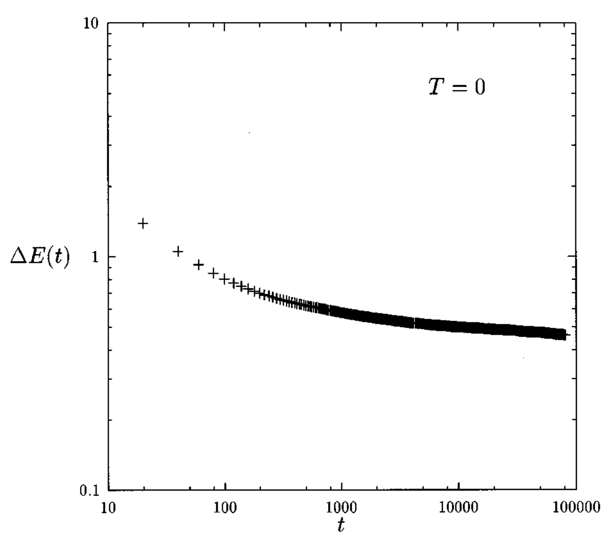

FIG. 1. Relaxation of the excess energy per site ΔE for a zero-temperature quench.

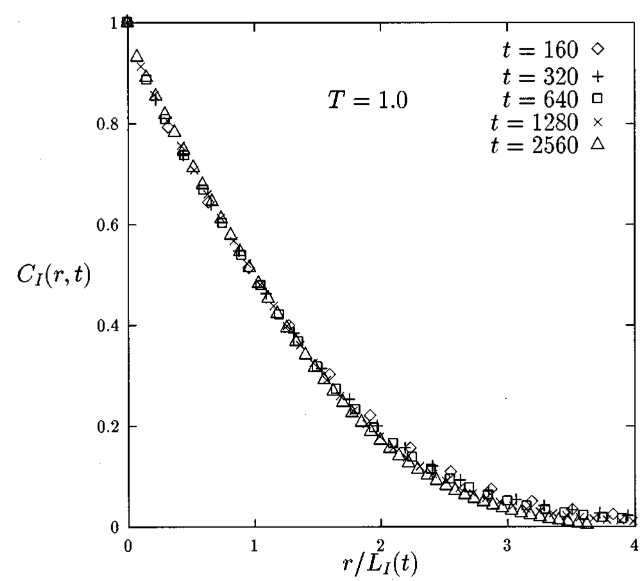

FIG. 2. Scaling collapse of the equal-time correlation functions for the Ising spin at $T = 1.0$ with $L_I(t) \sim t^{\phi_I}$, where $\phi_I \simeq 0.505$.

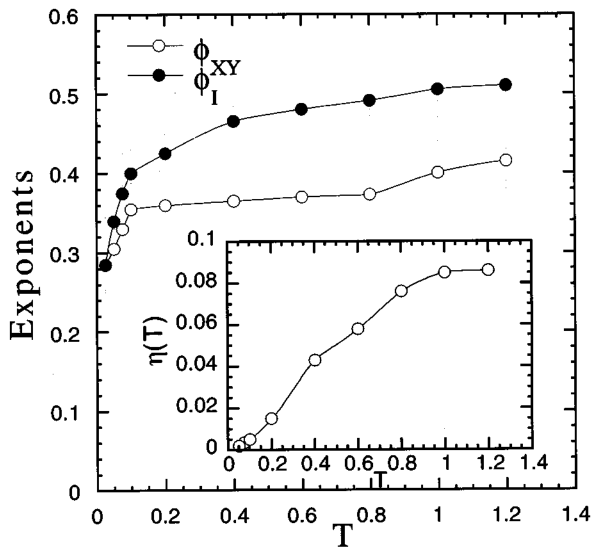

FIG. 3. Temperature dependence of growth exponents ϕ_{XY} and ϕ_I. Error bars are a few times the size of the symbols.

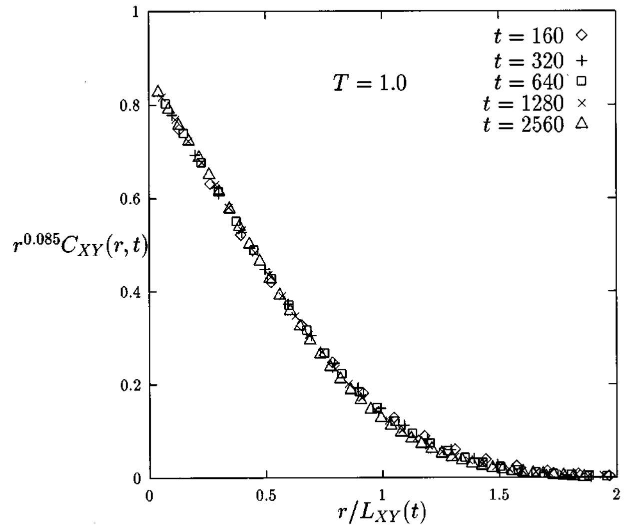

FIG. 4. Scaling collapse of the equal-time correlation functions for the XY spin at $T=1.0$ with $L_{XY}(t) \sim t^{\phi_{XY}}$, where $\phi_{XY} \simeq 0.4$.

lected: (i) rotation of the XY phase angle by a random amount, leaving the Ising spin unflipped, and (ii) rotation of the XY phase angle by a random amount *and* Ising spin flip.

Simulations were carried out on a square lattice of linear size $L=200$. The results presented are averages over 40–60 different random initial configurations. In order to carry out a quantitative analysis on the kinetics, we measure the equal-time correlation functions and autocorrelation functions for both XY and Ising order parameters. In addition to these quantities, we also measured the total length of Ising domain walls and the total number of the corners of the Ising domain walls to examine a possible morphological change.

III. SIMULATION RESULTS AND DISCUSSION

One of the most important characteristics in the ordering dynamics of a coupled XY-Ising model is the mutual pinning of vortices and Ising domain walls, as can be seen from the snapshots of the morphology of the system (Fig. 8). Now the XY ordering proceeds via coarsening and decay of the vortices and Ising ordering through the decay of the domain walls. Since the morphology shows mutual pinning between the two kinds of topological defects, we expect that a nontrivial growth law would result for the ordering for each order parameter from the pinning effect, which indeed is seen to be the case from the simulation results.

For the case of zero-temperature quench, we find that the system is driven into a metastable state and the ordering does not proceed any further. This can be best seen in the relaxation of the excess energy per site $\Delta E \equiv E(t) - E_0$, $E_0 = -4$ being the ground-state energy per site. As Fig. 1 shows, it saturates into some nonzero value, indicating that the system falls into a metastable configuration. Similar freezing behavior has also been observed in the FFXYM on a square lattice [9]. It is observed that this freezing is removed by a thermal fluctuation.

For a finite-temperature quench, in order to check the dynamic scaling and find the growth rate of the ordering processes, we first tried to collapse the Ising order parameter correlation functions $C_I(r,t)$ with a length scale $L_I(t)$, which is defined as $C_I(r=L_I(t),t)=1/2$ for a given time t. This gives a good data collapse for a given quenching temperature, as demonstrated in Fig. 2. This means that the equal-time Ising correlation function satisfies a simple dynamic scaling of the form $C_I(\vec{r},t) = f_I(r/L_I(t))$. As one can expect, the Ising length scale $L_I(t)$ shows a power-law growth in time of the form $L_I(t) \sim t^{\phi_I}$, but the growth exponent ϕ_I shows a temperature dependence, as seen in Fig. 3: it rapidly grows at low temperatures and saturates to the usual Ising exponent $\phi_I = 1/2$ at high temperatures.

Since the XY spin ordering is quasi-long-ranged, one expects a critical dynamic scaling for the XY spin correlation functions of the form $C_{XY}(\vec{r},t) = r^{-\eta} f_{XY}(r/L_{XY}(t))$, where $\eta(T)$ is the critical exponent for the equilibrium correlation at temperature T. Since an analytic expression is not available for η, assuming a power-law growth of the length scale $L_{XY}(t) \sim t^{\phi_{XY}}$, we adjust two parameters η and ϕ_{XY} to get the best scaling collapse. Figure 4 shows such a scaling collapse for $C_{XY}(r,t)$ at $T=1.0$ and the temperature dependence of the exponent $\eta(T)$ obtained from scaling collapse is shown in the inset of Fig. 3. Just as in the case of Ising domain growth, the XY growth exponent ϕ_{XY} quickly increases with temperature in the low-temperature region and then remains almost temperature independent with $\phi_{XY} \simeq 0.38$ for a broad range of temperatures. One might ask why the XY growth exponent remains considerably smaller than that of the pure XY model in two dimensions. This appears to be due to the pinning of point vortices near Ising domain walls. That is, the motion of vortices is strongly restricted by the presence of nearby Ising domain walls and hence the relaxation dynamics of point vortices is no longer the same as in the case of the pure XY model. In order to explain quantitatively the specific value of $\phi_{XY} \simeq 0.38$, we would have to understand the detailed mechanism of pinning interaction and the decay processes of the defects, in which we have not succeeded yet.

Let us turn to the low-temperature behavior of the growth exponents. Quite often, it is a rather difficult and subtle task

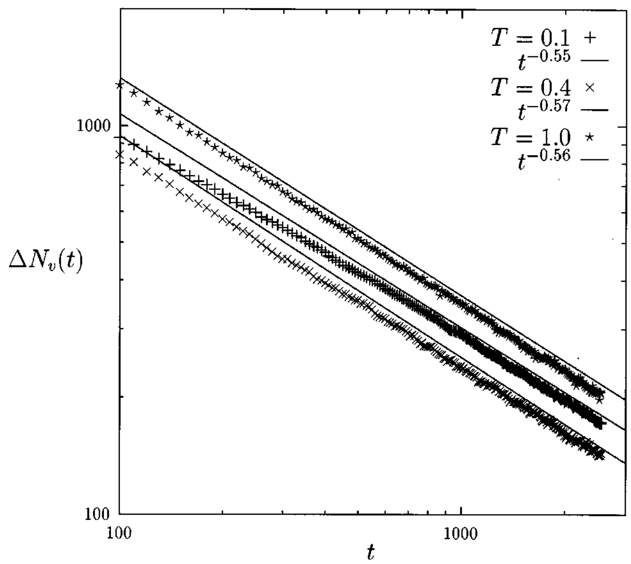

FIG. 5. Residual vortex number $\Delta N_v(t)$ of the XY spin versus time in a log-log plot at temperatures $T=0.1$, 0.4, and 1.0.

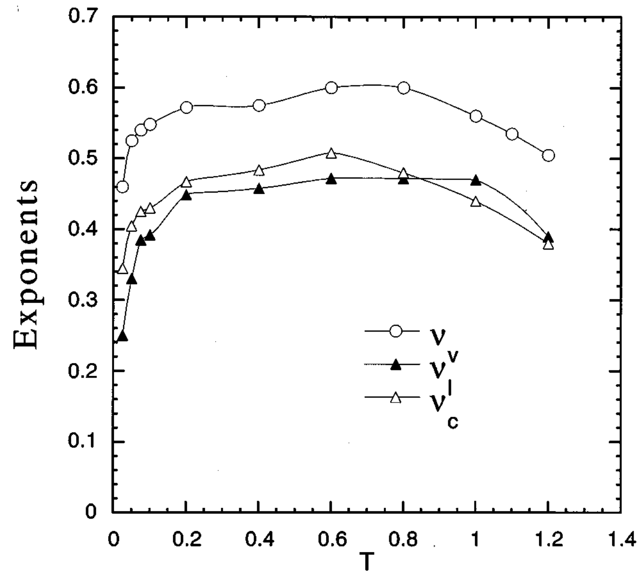

FIG. 6. Temperature dependence of various exponents ν_v, ν_c, and ν_l. Error bars are a few times the size of the symbols.

to determine the domain growth exponent at low temperature for an ordering system especially when the system exhibits a freezing behavior at zero temperature. As shown by Lai, Mazenko, and Valls (LMV) [23], for a system where the zero-temperature freezing is caused by local energy barriers that are independent of the size of ordered domains (a class II system according to LMV's classification), the typical behavior of the average domain size $L(t)$ goes as $L(t)\sim L_0+A(t/\tau(T))^{\phi}$, where $\tau(T)\simeq\tau_0\exp(E_0/T)$, with E_0 representing a barrier activation energy and A and τ_0 being weakly temperature-dependent quantities. L_0 is a length scale related to the typical frozen domains at $T=0$. Therefore, at low temperature ($T\ll E_0$), the characteristic time scale $\tau(T)$ becomes very large and it is very hard and almost impossible to reach numerically the time regime for the correct determination of the late-time growth exponent ϕ. In practice, almost inevitably, the measured exponents are underestimated compared to the true asymptotic values. In the present coupled XY-Ising model, a further complication arises from the continuous O(2) symmetry in addition to the Ising symmetry and from the fact that the XY order parameter itself develops into a quasiordered state via a quasiordering process. It is not clear at all, at this point, how to implement the renormalization-group analysis for our system, analogous to that of LMV. Due to these theoretical uncertainties, we have not attempted any detailed numerical or theoretical analysis of the type of LMV to our system. Here the most important question is whether the low-temperature ordering behavior of the system belongs to class II in LMV's classification or to a newer class, not discussed by LMV, which probably includes the FFXYM that shows quite convincingly a genuine temperature-dependent growth exponent at low temperatures. At this point, we should leave the answer for this question to further analysis.

There exists another time-dependent length scale that can be drawn from the time dependence of the distribution of the XY point vortices, that is, the average separation between point vortices. Since the quasiordering of the XY order parameter corresponds to the decay processes of the point vortices, this length scale must be closely related to the size of the ordered region for the XY degrees of freedom. Rigorously, we must deal with the residual vortex number $\Delta N_v(t)=N_v(t)-N_v(\infty)$, where $N_v(\infty)$ is the equilibrium vortex number at a given temperature. Figure 5 shows the excess vortex number for various temperatures where we can see a power-law behavior $\Delta N_v(t)\sim t^{-\nu_v}$ with the exponents ν_v varying weakly with the temperature as shown in Fig. 6. Interestingly enough, throughout the temperature range, the growth rate of the length scale $L_v(t)$ defined as $L_v(t)\sim 1/\sqrt{\Delta N_v(t)}$ does not coincide with that of $L_{XY}(t)$. For example, at $T=0.4$, we find $L_v(t)\sim t^{0.28}$, in contrast to $L_{XY}(t)\sim t^{0.36}$. We may interpret this discrepancy, at least qualitatively, in the following way. The fact that

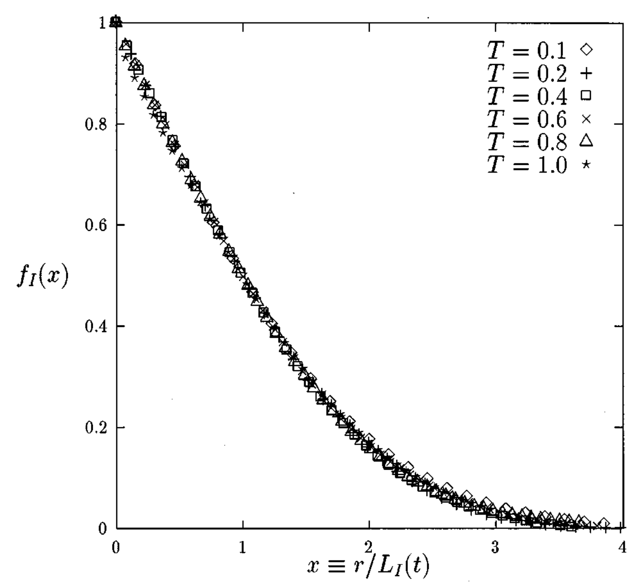

FIG. 7. Ising scaling functions $f_I(x)$ for various temperatures. The data plotted for each temperature are the rescaled Ising correlation function at $t=2560$.

$L_v(t) \sim 1/\sqrt{\Delta N_v(t)}$ grows more slowly than $L_{XY}(t)$ implies that the point vortices are not completely randomly distributed but that there exists some sort of clustering of point vortices so that the average separation between these clusters of point vortices actually corresponds to the length scale L_{XY}. One obvious possibility for this clustering behavior would be the effect of pinning of vortices near the Ising domain walls that would hinder the motion of vortices in the direction away from the domain walls. Since we also have to take into account the fact that XY ordering is a quasiordering process, we expect that the corresponding equilibrium exponent η also has to be considered in the above arguments. In spite of this theoretical caveat, the above argument appears to corroborate our numerical result that the Ising and XY domains grow with different exponents and indicate that there exist multiple length scales in the relaxation and ordering kinetics of our model system.

The Ising scaling function $f_I(x)$, where $x \equiv r/L_I(t)$ is shown in Fig. 7 for various temperatures. They all collapse onto a single curve even though the numerical values of the Ising growth exponents, especially at low temperatures, are temperature dependent. This, in turn, coincides with the scaling function for the pure Ising model in two dimensions.

In order to examine a possible morphological change, as observed in the FFXYM, we plot the snapshots of typical configurations for a quench to the temperatures $T=0.1$, 0.6, and 1.0, respectively, in Fig. 8. We see that while at low temperature ($T=0.1$), the domain walls become faceted at

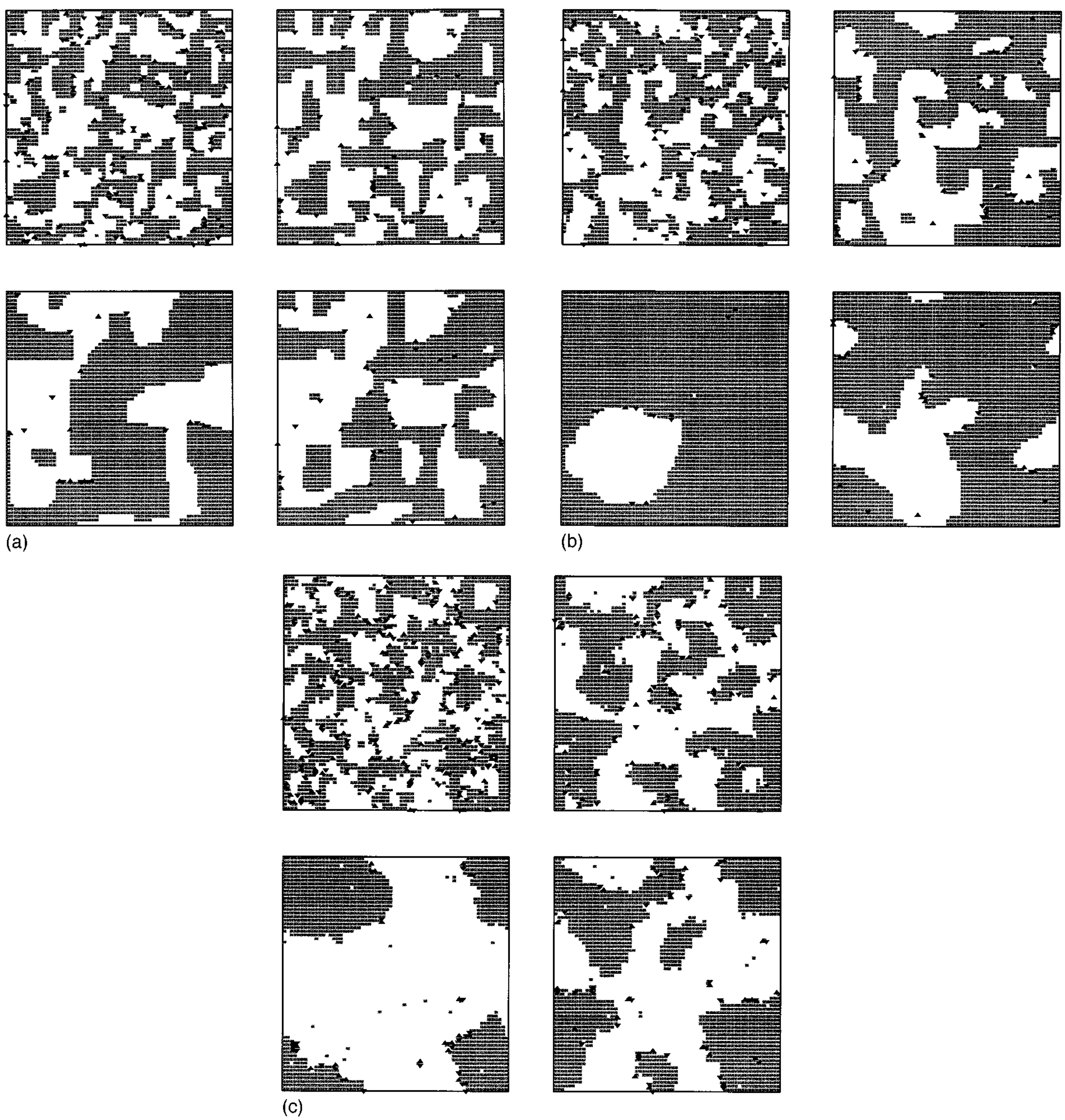

FIG. 8. Snapshots of configurations for Ising domains and XY spin vortices at (a) $T=0.1$, (b) $T=0.6$, and (c) $T=1.0$. In each set, figures represent the snapshots taken at $t=40$, 160, 640, and 2560, respectively, clockwise from the top left. Ising domains are denoted by different shades representing the different sign of the Ising spins. Up and down triangles represent vortices and antivortices respectively.

large length scales, the domain walls become rougher at high temperature ($T=1.0$). Note that the ordering is slower for lower temperature, consistent with the temperature dependence of ϕ_I obtained from scaling collapse of correlation functions.

For a more quantitative understanding of these morphological features, we calculated the time dependence of the total number of corners (N_c) and the total length (N_l) of Ising domain walls. Simulations show that these quantities decay in time toward their equilibrium values with a power law, i.e., $N_c(t)-N_c(\infty)\sim t^{-\nu_c}$ and $N_l(t)-N_l(\infty)\sim t^{-\nu_l}$. The temperature dependence of these exponents are shown in Fig. 6 together with ν_v. If we have $\nu_c>\nu_l$, then the total number of corners decays faster than the total length of line defects (domain walls), implying that the average separation between neighboring corners increases indefinitely in time, that is, we get flat domain walls. On the other hand, if we have $\nu_c\simeq\nu_l$, then the average separation between neighboring corners will be kept constant, resulting in rough domain walls. Even though the snapshots exihibit the characteristic morphological changes as T is increased from low to high temperature, we do not feel that we can make a definitive statement concerning the existence of the finite-temperature roughening transition from the numerical value of these exponents shown in Fig. 6. This question also seems to be related to the question as to the nature of the low-temperature growth kinetics, namely, whether the low-temperature barrier activation energy is independent of the average domain size or dependent on it. In this connection, we have to reconsider the fact that point vortices are mostly pinned near Ising domain walls either near the corners or along the sides of the domain walls. One important point to note, however, is that not all the geometric corners of the domain walls have pinned vortices on them. This is in contrast to the case of the FFXYM, where every corner of chiral domain walls corresponds to a vortex with fractional charge of 1/4. In this case of the FFXYM, we can argue similarly, as done by Uimin and Pimpinelli [24], that it is possible to have a finite-temperature roughening transition of Ising domain walls due to KT-type unbinding of fractional-vortex pairs because the fractional vortices can be identified as the geometric corners of Ising domain walls. In contrast, however, we cannot use this kind of argument straightforwardly in the present case of coupled XY-Ising model because some corners have vortex charges while others do not. Therefore, further extensive study is required to clarify this point.

We also have calculated the autocorrelation functions for both XY and Ising order parameters. Rather unexpectedly, we found that the power-law slope continues to increase in magnitude when plotting $A_{XY}(t)$ versus time in a log-log scale as shown in Fig. 9 at $T=0.6$, for example. This indicates that the spin autocorrelation function does not follow a power-law decay in time. Instead, as shown in the inset to Fig. 9, we found that it can be well fit by a stretched exponential behavior of the form $A_{XY}(t)\sim\exp(-ct^{\beta})$, with $\beta\simeq0.146$. Similar behavior for the XY spin autocorrelation function was found for all the other temperatures with an almost temperature-independent exponent β. The spin wave dominance within an Ising domain due to the pinning of vortices near the domain walls might be responsible for this stretched exponential relaxation. The one-dimensional XY model is another case where the spin autocorrelation function shows a stretched exponential behavior. For this model, it was analytically shown that a spin wave fluctuation gives rise to a stretched exponential decay of the spin autocorrelation with different value of $\beta=0.5$.

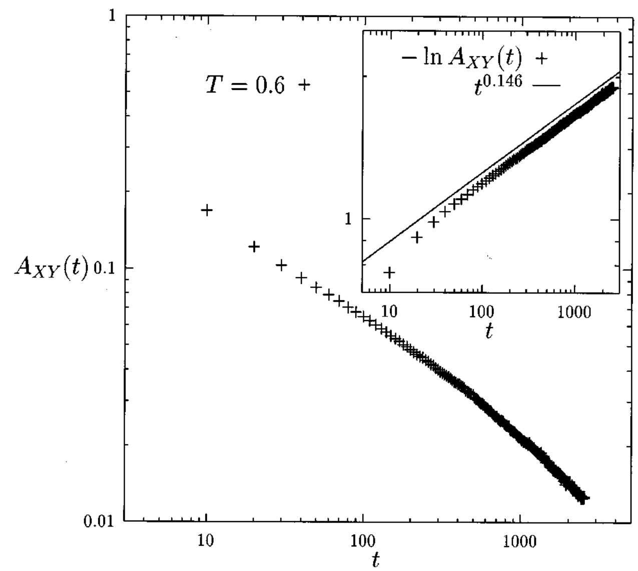

FIG. 9. Autocorrelation function of the XY spin order parameter versus time in a log-log plot at $T=0.6$. The inset is a stretched exponential plot for the same data.

The autocorrelation function $A_I(t)$ for the Ising order parameter showed a power-law behavior with $A_I(t;T)\sim L_I(t;T)^{-\lambda}\sim t^{-\phi_I\lambda}$ in time, as shown in Fig. 10 at $T=0.6$ for an example. The exponent λ varies from 1.1 to 1.25, but the statistics of the data is not good enough to determine whether the exponent λ is the same as that in the pure Ising model in two dimensions, which was analytically found to be 5/4 by Fisher and Huse [25].

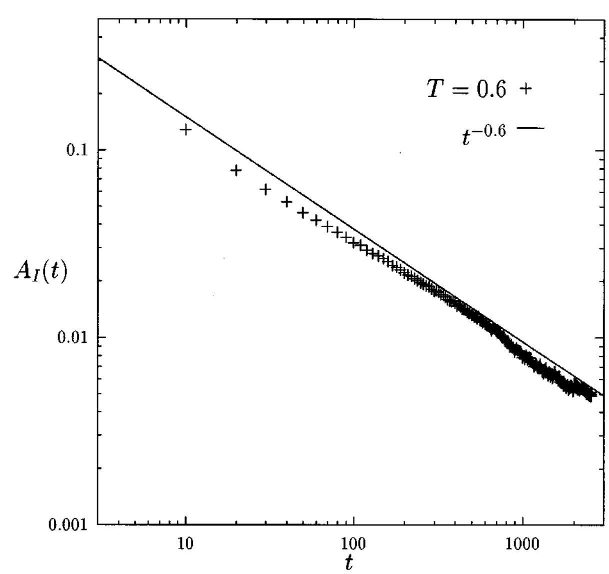

FIG. 10. Autocorrelation function of the Ising order parameter versus time in a log-log plot at $T=0.6$. Since $\phi_I(T=0.6)\simeq0.48$, $\lambda\simeq0.6/0.48\simeq1.25$.

IV. SUMMARY

In this work, we presented simulation results on the ordering dynamics of the coupled XY-Ising model in two dimensions. The ordering involves the annihilation processes of the two kinds of topological defects—Ising domain walls and XY spin vortices—and the interaction between these two defects. The pinning of vortices near Ising walls considerably reduces the growth rate of XY ordering and yields a stretched exponential relaxation in the autocorrelation function for the XY order parameter. Due to the presence of the multiple length scales in the ordering process, it would be interesting to probe the mutual correlations between the line and point defect densities.

ACKNOWLEDGMENTS

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