Ordering kinetics of two-dimensional O(2) models: Scaling and temperature dependence

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This paper presents simulation results on the phase-ordering kinetics of two-dimensional O(2) models. Both the time-dependent Ginzburg-Landau (TDGL) model and the fixed length spin XY model on a square lattice are studied using the Langevin dynamics approach. The equal-time correlation functions of the TDGL model at zero temperature quench are shown to scale best with the length scale form of $L(t) \sim [t/(\ln t)^{\gamma}]^{0.5}$, with $\gamma \simeq 0.7$, which is also consistent with the length scale derived from the energy-scaling argument, although with a slightly different value of γ. Critical dynamic scaling is satisfied for quenches to finite temperatures below T_{KT} (the Kosterlitz-Thouless transition temperature). Autocorrelation functions show reasonable agreement with the theoretically predicted behavior of $A(t) \sim L(t)^{-[\lambda_0+\eta(T)]}$, where λ_0 is the zero temperature exponent for the autocorrelation and $\eta(T)$ is the temperature-dependent exponent for the equilibrium correlation function.

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I. INTRODUCTION

Ordering kinetics of statistical thermodynamic systems quenched from a disordered phase to an ordered phase has long been a subject of intensive research [1]. Recent interest in this area focuses on systems with continuous global symmetries [2–15]. For these systems, depending on the dimensionality of the system and the number of components of the order parameter, various types of stable topological defects or structures such as vortices, strings, hedgehogs, and textures are possible and these defects act as disordering agents, greatly influencing the ordering dynamics of the system [7]. Among these systems, two-dimensional O(2) models [both the continuum time-dependent Ginzburg-Landau (TDGL) model and the discrete lattice XY model] have attracted much attention in recent years [8–15].

In spite of extensive numerical and theoretical efforts, the domain growth law and scaling properties of this system at zero temperature quench have not been completely settled, partly due to the apparent slow approach to the asymptotic growth law [14,15]. The correlation functions could be scale collapsed by a time-dependent length scale, but it did not coincide with the average length scale derived from the vortex density. Furthermore, most of the previous studies dealt with the case of zero temperature quenches only. However, for the O(2) model, the finite temperature quench is particularly interesting for the following reason. In equilibrium, the model exhibits a type of phase transition known as a Kosterlitz-Thouless (KT) transition at $T_{\rm KT}$ due to the unbinding of vortex-antivortex pairs [16]. Below $T_{\rm KT}$, the system has a quasi ordered phase that is characterized by a power law decay of order parameter correlation function for long distances. The critical exponent governing the power law decay decreases *continuously* down to zero temperature: the system is critical at equilibrium for all temperatures below $T_{\rm KT}$. In this sense, all finite temperature quenches below $T_{\rm KT}$ are critical quenches and therefore the temperature becomes relevent. Since the relaxation process here at finite temperature is an approach to a quasi-long-range order, it might be termed a "quasiordering process" [17].

In the present work, we investigate the phase-ordering kinetics of O(2) models in two dimensions for quenches to both zero and finite temperatures. The main results of the present work can be summarized as follows.

The order parameter correlation function obeys a critical dynamic scaling of the form

$$C(r,t) = r^{-\eta(T)} f\left(\frac{r}{L(t)}\right), \tag{1}$$

where $\eta(T)$ is the critical exponent for the equilibrium correlation function at temperature T and $L(t)$ is the average size of the ordered (or quasiordered) regions growing with time. For the case of zero temperature quench, the possibility of a tentative scaling violation has been addressed recently [15] based on the length scale derived from the density of defects (vortices). We show here that, following the energy scaling approach due to Rutenberg and Bray [18,19], the scaling hypothesis does in fact hold only if we use the length scale derived from the relation between the energy vs the length scale of the domain size. If we denote this length scale by $L_E(t)$, then we could fit $L_E(t)$ into the form $L_E(t) \sim [t/(\ln t)^{\gamma}]^{0.5}$ with $\gamma \simeq 0.75$. We emphasize the discrepancy between this length scale $[L_E(t)]$ and that from the vortex density $[L_V(t)]$ in the different logarithmic corrections (see Sec. III for more de-

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tails). The nonequilibrium exponent [20] associated with the autocorrelation function for zero temperature quench is in excellent agreement with the theoretical predictions made by Bray and Puri [4] and independently by Liu and Mazenko [5]: $A(t) \sim L(t)^{-\lambda_0}$, where $\lambda_0 \simeq 1.17$. For the case of finite temperature quenches, the simulation results are in reasonable agreement with the theoretically predicted behavior of $A(t) \sim L(t)^{-\lambda(T)}$, where $\lambda(T) = \lambda_0 + \eta(T)$.

This paper is organized as follows. In Sec. II we describe the Hamiltonian of the model, the associated Langevin dynamic equation, and the measured quantities. In Sec. III the results of the numerical simulations are presented in detail. Section IV summarizes the results.

II. MODELS

The Ginzburg-Landau Hamiltonian of the O(2) model is given by

$$H = \int d^2r[\tfrac{1}{2}(\nabla\vec{\phi})^2 + \tfrac{1}{4}(\vec{\phi}^{\,2} - 1)^2] \ , \tag{2}$$

where $\vec{\phi}$ is a two-component real vector field $\vec{\phi} = (\phi_1, \phi_2)$. The time evolution of the model is assumed to be governed by the model A dynamics appropriate to the nonconserved order parameter, of the form

$$\begin{aligned}\frac{\partial \phi_\alpha}{\partial t} &= -\frac{\delta H}{\delta \phi_\alpha} + \zeta_\alpha(\vec{r}, t) \\ &= \nabla^2\phi_\alpha + (1 - \vec{\phi}^{\,2})\phi_\alpha + \zeta_\alpha(\vec{r}, t), \quad \alpha = 1, 2\end{aligned} \tag{3}$$

where the thermal noise $\zeta_\alpha(\vec{r}, t)$ is white Gaussian with zero mean and with variance satisfying the detailed balance at temperature T,

$$\langle \zeta_\alpha(\vec{r}, t)\zeta_\beta(\vec{r}\,', t')\rangle = 2k_BT\delta_{\alpha\beta}\delta(\vec{r} - \vec{r}\,')\delta(t - t'). \tag{4}$$

We have also studied the dynamics of the hard spin XY model on square lattice whose Hamiltonian is given by

$$H = -J\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j = -J\sum_{\langle ij\rangle} \cos(\theta_i - \theta_j) \ , \tag{5}$$

where J is the interaction strength and θ_i is the phase angle of the spin at site i; $\vec{S}_i \equiv (\cos\theta_i, \sin\theta_i)$ and the sum is over nearest neighbors. The corresponding dynamic equation we use is of the form

$$\frac{\partial \theta_i}{\partial t} = -\frac{\delta H}{\delta \theta_i} + \zeta_i(t), \quad i = 1, \ldots, N^2 \ , \tag{6}$$

where the thermal noise $\zeta_i(t)$ satifies

$$\langle \zeta_i(t)\zeta_j(t')\rangle = 2k_BT\delta_{ij}\delta(t - t'). \tag{7}$$

Both (6) and (7) are numerically integrated in time using Euler's method with the integration time step $\Delta t =$ 0.05–0.1 and we use the discrete lattice Laplacian in (3) with the mesh sizes given by $\Delta x = \Delta y = 1$. Periodic boundary conditions on both lattice directions are employed. Simulations were carried out on square lattices of linear size $N = 256$ for the case of the hard spin XY model, while for the case of O(2) the TDGL model with a lattice size of $N = 800$ was used for zero temperature quench and $N = 400$ for finite temperature quenches. The final results are obtained from averages over 30 different random initial configurations. Main quantities of interest are expressed in terms of the O(2) TDGL model as follows: (i) excess energy relaxation (at zero temperature) is defined as

$$\Delta E(t) = \frac{1}{N^2}\left\langle \sum_{i,\hat{n}}[\tfrac{1}{2}(\vec{\phi}_{i+\hat{n}} - \vec{\phi}_i)^2 + \tfrac{1}{4}(\vec{\phi}_i^{\,2} - 1)^2] \right\rangle \ , \tag{8}$$

where $\langle\,\rangle$ denotes an average over random initial configurations, (ii) the equal time correlation function

$$C(r, t) = \frac{1}{N^2}\left\langle \sum_i \vec{\phi}_i(t) \cdot \vec{\phi}_{i+r}(t) \right\rangle \ ; \tag{9}$$

(iii) the two-time autocorrelation function

$$\tilde{A}(t, t') = \frac{1}{N^2}\left\langle \sum_i \vec{\phi}_i(t) \cdot \vec{\phi}_i(t') \right\rangle, \tag{10}$$

where we only measure correlations with initial configurations, namely, $t' = 0$,

$$A(t) \equiv \tilde{A}(t, 0) \ ; \tag{11}$$

and (iv) the number of vortices at time t is $N_V(t)$.

It is straightforward to write down the corresponding quantities in the hard spin XY model on square lattices. The results of simulations will be presented mainly in terms of O(2) TDGL model, but when necessary we will compare the results with those obtained from the hard spin XY model on square lattices.

III. SIMULATION RESULTS

A. Zero temperature quench

Here we present simulation results on the O(2) TDGL model for the case of zero temperature quench. The main objective here is to check whether the scaling assumption holds in this system and to obtain the domain growth law. Recently a tentative scaling violation in the two-dimensional O(2) model has been suggested by Blundell and Bray [15]. Their suggestion is based on the scaling relation $\rho(t) \sim L^{-2}(t)$, where $\rho(t)$ is the defect number density. Using this relation, when the equal-time correlation function $C(r, t)$ was scaled with $r\rho^{1/2}(t)$, the data collapse failed. We note that there exists another scaling relation that relates the excess energy density to the domain size. We may reexamine the equal-time correlation functions in terms of the length scale derived from the energy scaling relation. The excess energy vs time is shown in Fig. 1. We see that the excess energy continues to decay toward zero and hence there is no sign of freezing in for the case of the continuous O(2) TDGL model in two dimensions, in contrast to the case of the hard spin XY

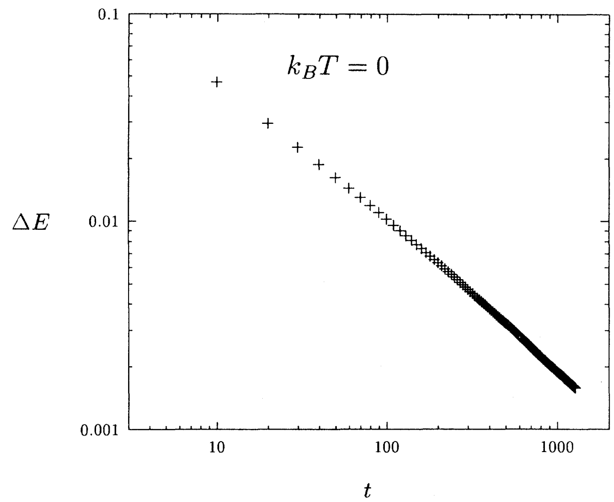

FIG. 1. Time dependence of the excess energy for the O(2) TDGL model at zero temperature. The lattice size is 800×800 and the results are averages over 30 different random initial configurations.

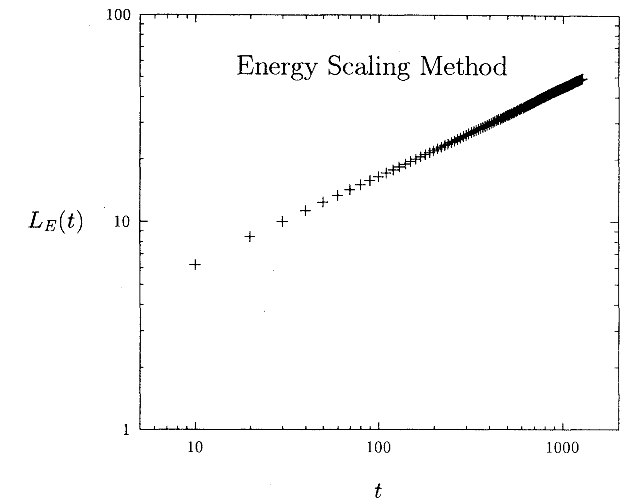

FIG. 2. Time dependence of the length scale $L_E(t)$ obtained from the relation [Eq. (16)] between the energy density (Fig. 1) and the domain size scale.

model (first observed by Bray and Humayun [11]), where the excess energy is seen to decay toward some nonzero value and the ordering does not proceed any further due to lattice pinning of vortices.

Following Bray and Rutenberg [18], it is easy to prove that in (2) the excess energy is dominated by the gradient term and hence

$$\Delta E(t) \sim \left\langle \int d^2r(\nabla\vec{\phi})^2 \right\rangle \sim \int d^2kS(k,t)k^2 \ , \qquad (12)$$

where $S(k,t)$ is the Fourier transform of the equal-time correlation function $C(r,t)$. If the scaling hypothesis holds, namely,

$$C(r,t) = f\big(r/L(t)\big) \ , \qquad (13)$$

where $L(t)$ is the average size of ordered regions at time t, then

$$S(k,t) = L^2(t)g(kL(t)). \qquad (14)$$

Putting (14) back into (12), one obtains

$$\Delta E(t) \sim L^{-2}(t) \int d^2xx^2g(x) \ , \qquad (15)$$

where the scaling function $g(x)$ behaves like $g(x) \sim x^{-4}$ for $x \gg 1$ due to the presence of vortices; this is known as the generalized Porod law [4–7,18]. This makes the integral in (15) logarithmically divergent for large x, yielding

$$\Delta E(t) \sim L^{-2}(t)\ln[L(t)/\xi] \ , \qquad (16)$$

where $\xi \simeq 1$ is the size of a vortex core. We can obtain another equation relating the energy dissipation to $L(t)$ and dL/dt [18]. By combining this relation with (16), Rutenberg and Bray could derive scaling laws for the domain growth. However, in the case of O(2) model in two dimensions, the additional relation becomes degenerate with (16) and hence the scaling law cannot be determined in this way. Here we have, from simulations, the time dependence of the excess energy. Therefore, we decided to solve (16) directly for $L(t)$ up to an overall factor, using the excess energy from simulations and then try to scale the equal-time correlation functions with the numerically determined solution $L(t) = L_E(t)$ in order to test whether the scaling hypothesis is really consistent. Figure 2 shows such a solution with the core size $\xi = 1$. The rescaled data on equal-time correlation $C(r,t)$ collapse nicely except for the early-time regime ($t \leq 20$), which is shown in Fig. 3. Hence we see that the scaling hypothesis (13) is indeed consistent at least with the relation between the excess energy and the domain size. In

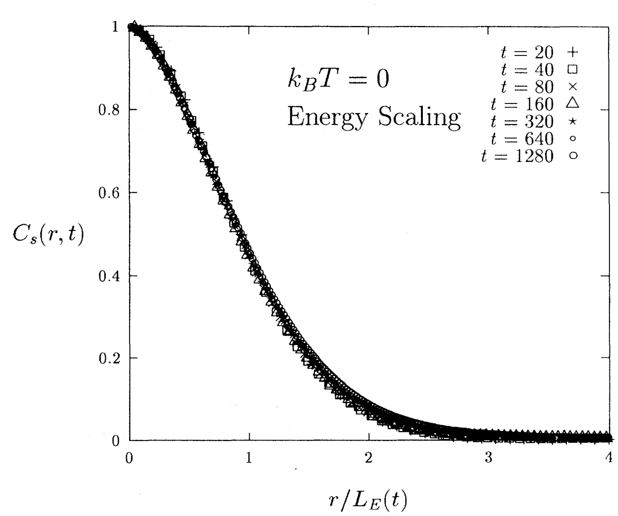

FIG. 3. Scaling collapse of the equal-time correlation functions for the O(2) TDGL model at zero temperature using the length scale $L_E(t)$ as shown in Fig. 2.

order to extract the growth law for the domain size, we first tried a pure power law fit, which gave $L_E(t) \sim t^{0.44}$. Figure 4(a) shows the scaling collapse of the $C(r,t)$ using the corresponding pure power law for the domain size. But notice that, even though the power law fit is quite good in the long-time regime, the fit is not good in the shorter-time scale. As another form of the growth law, we attempted a growth law of the form

$$L_E(t) \sim [t/\ln(t)^\gamma]^{1/2}. \tag{17}$$

This form is motivated by the expectation that the true *asymptotic* growth law probably would be $L(t) \sim t^{1/2}$ in the very-long-time regime, but that there would exist some logarithmic corrections. Plotting $L_E(t)/t^{1/2}$ versus $\ln(t)$ in logarithmic scale yields $L_E(t) \sim [t/\ln(t)^\gamma]^{1/2}$ with $\gamma \simeq 0.75$. Independently of this, we tried to collapse the equal-time correlation functions by the form (17), which is shown in Fig. 4(b), where we get the best collapse for $L(t) \sim [t/\ln(t)^{\gamma_1}]^{1/2}$ with $\gamma_1 \simeq 0.7$. This is in reasonable agreement with (slightly less than) the corresponding exponent value from $L_E(t)$. Note that the scaling collapse with this form with logarithmic correction is much better than that with the form of a pure power law, especially in the early-time regime. Therefore, the growth may be viewed as diffusive with a correction of nontrivial logarithmic power, even though it is very difficult numerically (based on simulation results for finite time window) to differentiate between a pure power law of, say, $L(t) \sim t^{0.44}$ and diffusive growth with logarithmic corrections.

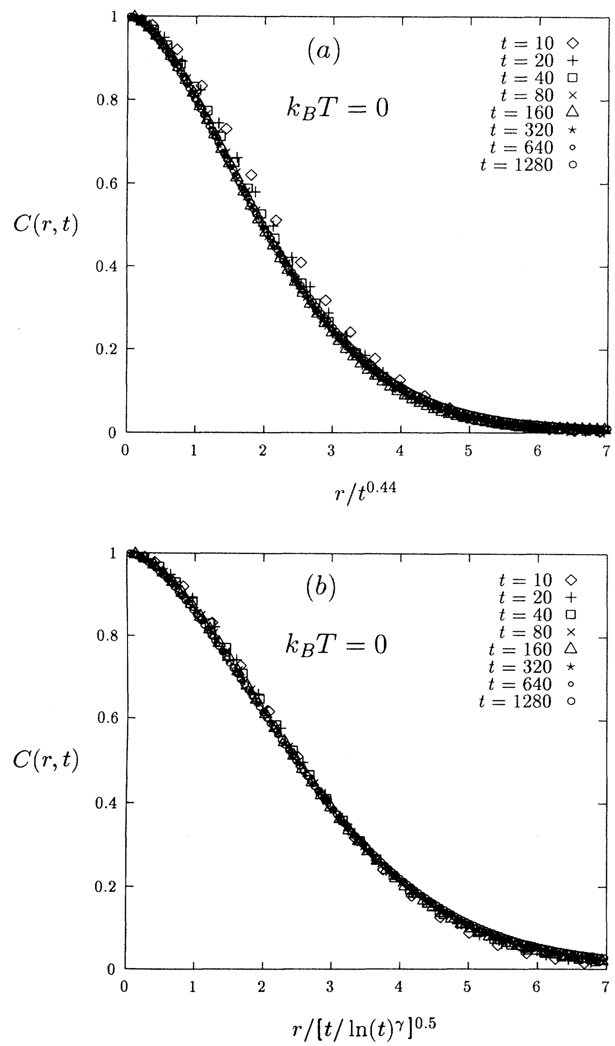

FIG. 4. Scaling collapse of the order parameter correlation functions for the O(2) TDGL model at zero temperature using (a) a pure power law form of domain growth with $L(t) = t^{0.44}$ and (b) a diffusive form with logarithmic corrections $L(t) = \{t/[\ln(t)]^\gamma\}^{1/2}$ with $\gamma = 0.7$.

Going back to the relation between the defect number density and the length scale, there are two important ingredients in the derivation of this relation. First, the scaling assumption (13) and the generalized Porod law gives

$$\begin{aligned} S(k,t) &= L^2(t)g(kL(t)) \\ &\sim L^2(t)[kL(t)]^{-4} \\ &\sim L^{-2}(t)k^{-4} \quad \text{for } kL \gg 1. \end{aligned} \tag{18}$$

Second, the singular part of the equal-time correlation function is shown to be [19]

$$C_{\text{sing}} = \rho(t)r^2\ln[r/L(t)], \tag{19}$$

which leads to $S(k,t) \sim \rho(t)k^{-4}$ for $kL(t) \gg 1$. This, compared with (18), yields the scaling relation $\rho(t) \sim L^{-2}(t)$. We have plotted in Fig. 5(a) the decay of the number of total defects (both vortices and antivortices) $N_V(t)$, which is proportional to the defect number density. Motivated by the possibility of aymptotic growth of $L(t) \sim t^{1/2}$, one may assume an ansatz form of $N_V(t) \sim \ln^\mu(t)/t$. Plotting $N_V(t)t$ vs $\ln(t)$ [Fig. 5(b)] gives $\rho(t) \sim \ln(t)/t$, that is, we have $\mu = 1$, as was argued by Rutenberg and Bray [18].

It is interesting to point out that this form of the time dependence of the defect density $\rho(t) \sim \ln(t)/t$ is also observed, in various contexts, in the problem of an annihilating random walk [21] and in the relaxation dynamics in the two-dimensional Ising model with local gauge symmetry [22], where neighboring frustrated plaquettes annihilate each other. Using the numerically determined $L(t) = L_E(t)$ from the excess energy relaxation, one can directly obtain the relation between $\rho(t)$ and $L(t)$. Figure 5(c) provides such a plot. For the late-time regime, measuring the slope yields $\rho(t) \sim L^{-1.93}(t)$. Also shown is a line with slope -2 for comparison. One can see a discrepancy between the two, which is the reason for the apparent failure of the scaling collapse of $C(r,t)$ in terms of $L_V(t)$. It is not yet clear why the scaling collapse does work with $L(t) = L_E(t)$ but not with $L_V(t)$. But we conjecture that the long-range logarithmic interaction between vortices and antivortices might generate a few length scales with the same asymptotic behavior but with different logarithmic corrections. For example, we may consider the average size of a vortex-antivortex pair and the average distance between neigh-

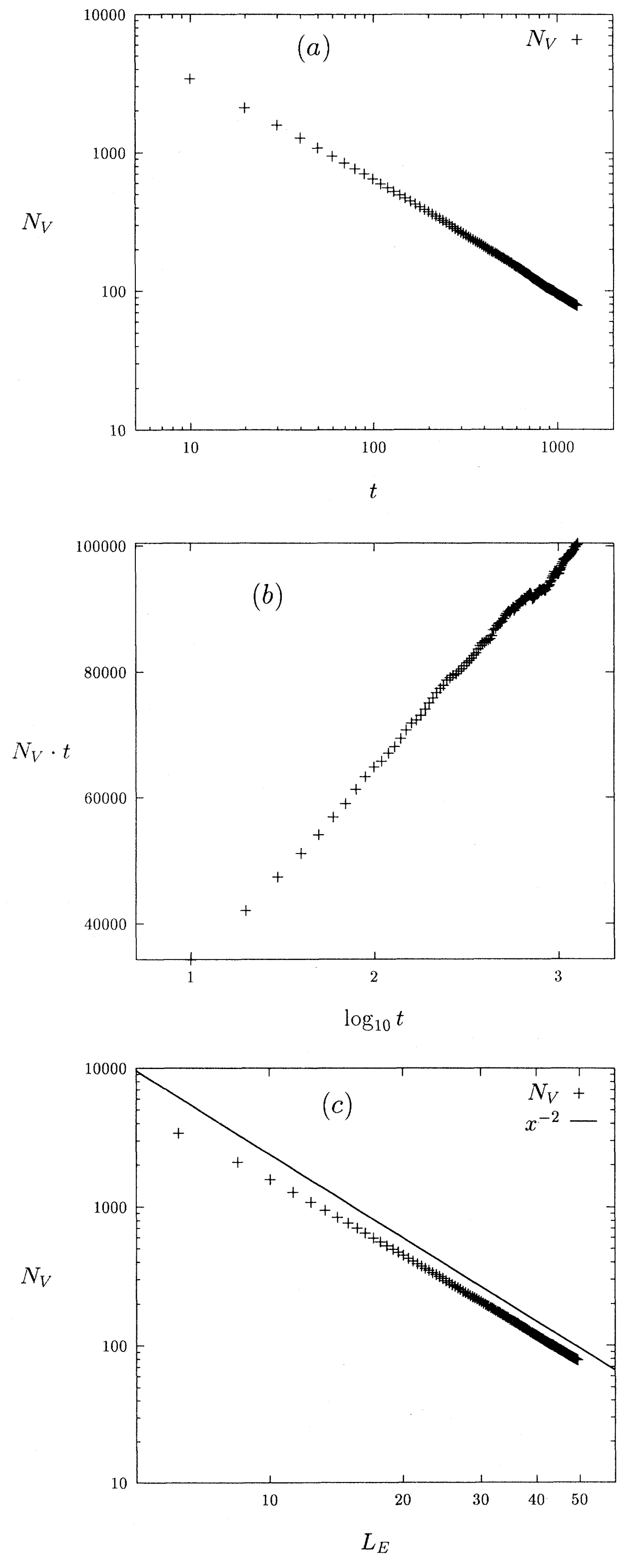

FIG. 5. (a) Time dependence of the total defect (vortex and antivortex) number for the O(2) TDGL model at zero temperature. (b) $N_V(t)t$ vs $\ln(t)$ shows straight line confirming $N_V(t) \sim \ln(t)/t$. (c) The total defect number vs the length scale $L_E(t)$, where the solid line represents a power law with slope -2. We can see a discrepancy between the two.

boring vortex-antivortex pairs. Individual vortex and antivortex within a pair interact logarithmically, while two neighboring vortex-antivortex pairs will interact effectively via a dipole-dipole interaction, which is much weaker than a logarithmic interaction. Therefore, we may expect that, due to this strong correlation between the vortex and the antivortex within a pair, the time dependence of the average size of a vortex-antivortex pair and that of the average distance between neighboring vortex-antivortex pairs will possibly have the same asymptotic behavior but with different logarithmic corrections. This may be the cause of the subtle logarithmic correction appearing in the length scale $L_E(t)$. More detailed simulations and analysis will be necessary to resolve this question.

The dependence of the autocorrelation function on $L(t)$ is determined in a similar fashion as above and is shown in Fig. 6, where we use $L(t) = L_E(t)$. We obtain from Fig. 6 $A(t) \sim L^{-\lambda_0}(t)$ with $\lambda_0 \simeq 1.171$, which is in excellent agreement with the result obtained from Mazenko's theory and the $1/n$-expansion result due to Newman and Bray [23].

B. Finite temperature quench

In the two-dimensional O(2) model, the system becomes critical at all temperatures below $T_{\rm KT}$. At equilibrium, the correlation function behaves as $C_{\rm eq}(r) \sim r^{-\eta(T)}$. Therfore one expects that the quasiordering dynamics at finite temperature quenches below $T_{\rm KT}$ will not be governed by the zero temperature fixed point. Instead, the zero temperature dynamic scaling for the equal-time correlation function (13) and (14) will be generalized, in the case of finite temperature quench, to

$$C(r,t) = r^{-\eta(T)} f(r/L(t,T)) \qquad (20)$$

and

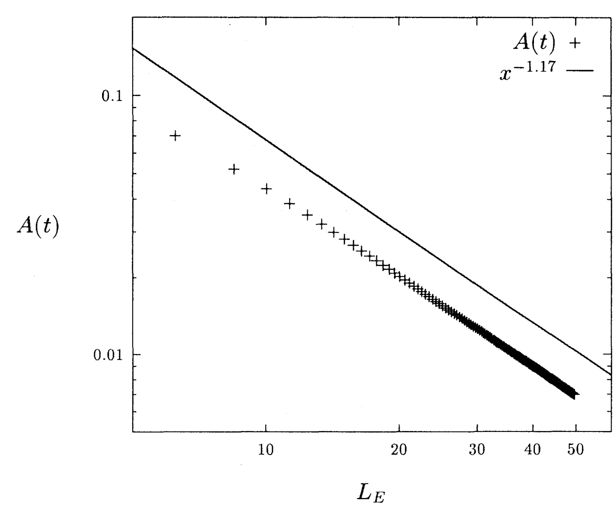

FIG. 6. Autocorrelation function of the order parameter plotted in terms of the length scale $L_E(t)$ for the O(2) TDGL model at zero temperature, which shows excellent agreement with the theoretical predictions $\lambda_0 \simeq 1.17$.

$$S(k,t) = L^{2-\eta(T)} g(kL(t,T)) \; , \qquad (21)$$

respectively. In (20) and (21) the exponent $\eta(T)$ is the critical exponent for the equilibrium correlation function. A rough value of T_{KT} could be determined by dynamic simulations as the temperature above which the ordering process does not proceed indefinitely but stops at some finite length scale. We could get $T_{\mathrm{KT}} \approx 0.42$. Figures 7(a) and 7(b) show examples of critical dynamic scaling, in the case of the O(2) TDGL model, for $k_B T = 0.2$ and 0.4, where we tried only a power law form of the growth law for the quasiordered domain $L(t,T) \sim t^{1/z(T)}$. The dynamic exponent $1/z(T)$ for different temperatures ranges between 0.41 and 0.44 when a power law fit is attempted. However, for the case of finite temperature quenches, we could not collapse the equal-time correlation functions using a growth law of diffusive form with logarithmic corrections. Also, it is fair to say that the quality of the scaling collapse at high temperatures is not as good as those at lower temperatures. We have also checked for the hard spin XY model on square lattices that the critical dynamic scaling of the form (20) holds [see Fig. 7(c)] and the temperature dependence of the exponent $\eta(T)$ is in good agreement with the theoretical prediction made by Villain [24]: $\eta(T) = \tau/2\pi + \tau^2/4\pi$, with $\tau \equiv T/J$.

For the autocorrelation function at finite temperatures, Fig. 8 shows the numerical results on its time dependence, for different temperatures. We can see that the power law slope tends to increase slightly at higher temperatures. Motivated by the case of zero temperature, we may set

$$A(t) \sim L^{-\lambda(T)}(t) \sim t^{-[\lambda(T)/z(T)]} \; . \qquad (22)$$

Theoretically, we may understand this behavior using the scaling assumption of the two-time correlation function. As a generalization of (21), the two-time correlation function may be written in the form

$$S(k,t,t') \equiv \left\langle \vec{\phi}(\vec{k},t) \cdot \vec{\phi}(-\vec{k},t') \right\rangle = L^{2-\eta}(t)[L(t')/L(t)]^{\lambda_0} h(kL(t),kL(t')), \quad t \gg t' \; . \qquad (23)$$

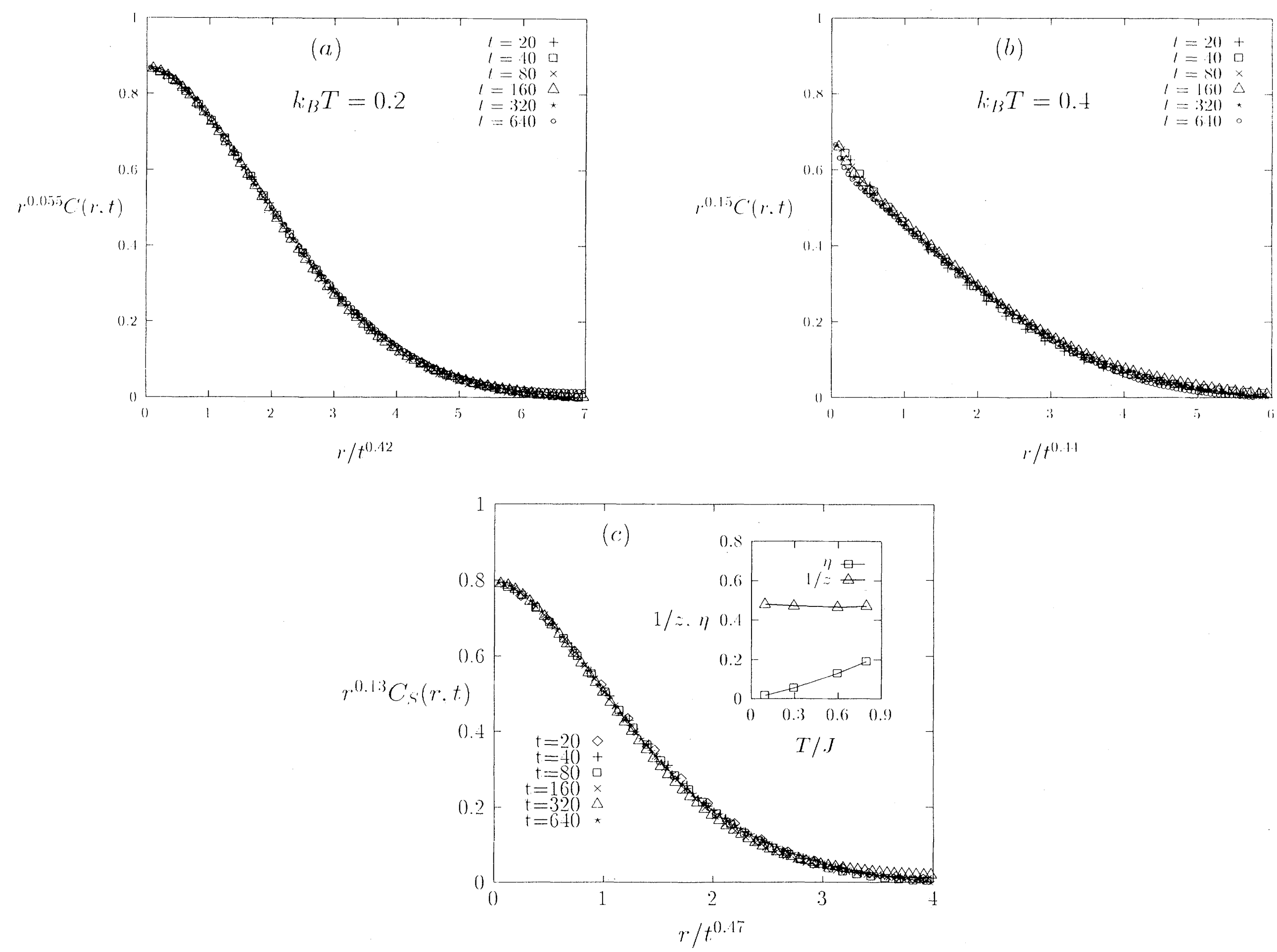

FIG. 7. Scaling collapse of the order parameter correlation functions for the O(2) TDGL model (400 × 400 lattice) at finite temperatures with (a) $k_B T = 0.2$, (b) $k_B T = 0.4$, and (c) similar scaling collapse of the order parameter correlation functions for the XY model on a square lattice (256 × 256) at temperature $k_B T = 0.6J$. The inset to (c) shows $1/z(T)$ and $\eta(T)$ for the XY model, where solid lines are only guides to the eye. A pure power-law form is used for the domain growth.

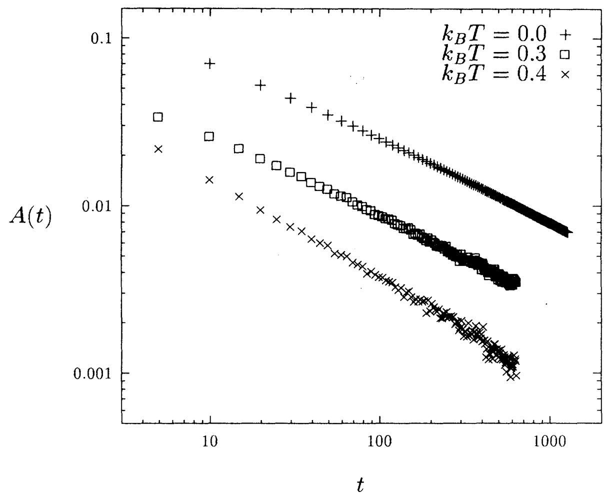

FIG. 8. Time dependence of the autocorrelation function of the order parameter for the O(2) TDGL model at different temperatures, which shows a slight increase in the power exponents as the temperature increases.

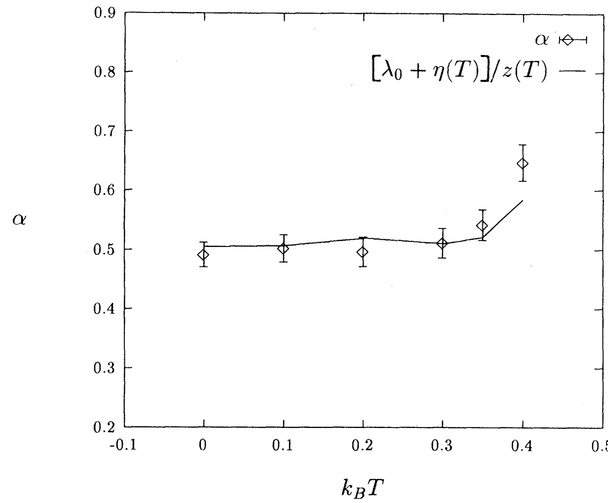

FIG. 9. Temperature dependence of the autocorrelation exponents $\alpha(T)$ as defined in the text. Diamonds are the exponents directly measured from the simulation results and the solid line represents the theoretical prediction based on Eqs. (22) and (24) in the text and those values of $\eta(T)$ and $1/z(T)$ obtained from the scaling collapse of the equal-time correlation functions of the order parameter.

The autocorrelation function is given by

$$A(t) = \int d^2kS(k,t,t_0) \sim L(t)^{-(\lambda_0+\eta)} , \qquad (24)$$

yielding $\lambda(T) = \lambda_0 + \eta(T)$. Figure 9 shows the simulation results of the power exponents $\alpha(T)$ defined through $A(t) \sim t^{-\alpha(T)}$ and the derived quantities $[\lambda_0 + \eta(T)]/z(T)$, where we use $\lambda_0 = 1.17$ and $\eta(T)/z(T)$ extracted from the scaling collapse of the equal-time correlation functions. We find reasonable agreement.

IV. SUMMARY

In this work, we presented simulation results and a detailed analysis on the ordering kinetics of the O(2) models in two dimensions, especially in terms of zero temperature scaling and temperature dependence. At zero temperature, the length scale derived from energy scaling argument was shown to give a good collapse of the equal-time correlation functions, although the length scale from the defect density does not. The domain growth law can be fitted into a diffusive form with logarithmic corrections of nontrivial power. Further study would be necessary to understand why this is so. In the case of finite temperature quenches, a critical dynamic scaling was satisfied for the equal-time correlation functions and the autocorrelation exponents showed a temperature dependence as predicted from the scaling hypothesis.

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