Phase ordering of two-dimensional XY systems below the Kosterlitz-Thouless transition temperature

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We consider quenches in nonconserved two-dimensional XY systems between any two temperatures below the Kosterlitz-Thouless transition. The evolving systems are defect free at coarse-grained scales, and can be exactly treated. Correlations scale with a characteristic length $L(t) \propto t^{1/2}$ at late times. The autocorrelation decay exponent, $\bar{\lambda} = (\eta_i + \eta_f)/2$, depends on both the initial and the final state of the quench through the respective decay exponents of equilibrium correlations, $C_{eq}(r) \sim r^{-\eta}$. We also discuss time-dependent quenches.

Phase-ordering kinetics is the study of the nonequilibrium process of equilibration after a rapid change of system parameters such as temperature or pressure [1]. Typically, the system is quenched from a high-temperature disordered phase to a low-temperature ordered phase. The problem is challenging because there are degenerate ground states competing to select the ordered phase and because the evolution of the order parameter is typically determined by a nonlinear partial differential equation. Indeed, there have been only a handful of exact solutions in phase-ordering systems (see [1]): nonconserved scalar and XY [O(2)] systems in one dimension, and both nonconserved and conserved spherical models in general dimensions. Typically, phase-ordering systems have singular topological defects (such as domain walls, vortex lines, or point defects) seeded from the disordered initial conditions. While the structure of singular defects can be used to extract the growth laws of characteristic scales through energy-scaling arguments [2], their singular nature makes exact solutions of correlation functions difficult. In fact, most of the exact solutions mentioned above do not involve singular defects: one-dimensional XY systems have only nonsingular topological textures [3], while spherical systems have no topological defects. It is natural, therefore, to consider other systems without topological defects.

In this paper, we consider the coarse-grained two-dimensional (2D) XY model below the Kosterlitz-Thouless transition temperature T_{KT}, where there are no free vortices [4]. For nonconserved dynamics we determine exactly the two-point correlations after a quench between any two temperatures at or below T_{KT}. We find scaling solutions characterized by a single time-dependent length $L(t) \sim t^{1/2}$ without the logarithmic factor $[L \sim (t/\ln t)^{1/2}]$ associated with quenches to states with free vortices (i.e., from above T_{KT}) [2,5]. We also measure autocorrelations for which the decay of the overlap with initial conditions is characterized by an exponent $\bar{\lambda}$ through $A(t) \sim L^{-\bar{\lambda}}$ [6–8]. For quenches to $T = 0$ we find $\bar{\lambda} = \eta_i/2$, where η_i characterizes the initial asymptotic spatial correlations through $C(r) \sim r^{-\eta_i}$. This agrees with the predictions of Bray *et al.* for quenches from a critical point to zero temperature [9]. For quenches between arbitrary temperatures below T_{KT} we find $\bar{\lambda} = (\eta_i + \eta_f)/2$, which depends on the initial *and* final states of the quench

[η_f characterizes the asymptotic *equilibrium* correlations at the final state through $C_{eq}(r) \sim r^{-\eta_f}$]. We also discuss quenches with arbitrary temperature histories, and show that asymptotic correlations and autocorrelations are independent of the early temperature history.

We consider overdamped, nonconserved, dissipative, "model A" dynamics with an equation of motion

$$\partial_t \vec{\phi} = -\Gamma \, \delta H / \delta \vec{\phi} + \vec{\xi}(\mathbf{x}, t), \qquad (1)$$

where $\vec{\phi}(\mathbf{x})$ is a two-component order parameter. The energy functional

$$H[\vec{\phi}] = \int d^2\mathbf{x} \left[\tfrac{1}{2}(\nabla \vec{\phi})^2 + V(\vec{\phi}) \right], \qquad (2)$$

has a potential with a symmetric global minimum at $|\vec{\phi}| = 1$, such as $V(\vec{\phi}) = V_0(\vec{\phi}^2 - 1)^2$. The thermal noise $\vec{\xi} = (\xi_1, \xi_2)$ is a Gaussian distributed with zero mean, with correlations determined by the fluctuation dissipation theorem $\langle \xi_i(\mathbf{x}, t) \xi_j(\mathbf{x}', t') \rangle = 2\Gamma k_B T \delta^2(\mathbf{x} - \mathbf{x}') \delta(t - t') \delta_{ij}$. Below the Kosterlitz-Thouless transition for the 2D XY model [4], any vortices present will be bound in oppositely charged pairs. We only consider correlations at distances much larger than the characteristic pair size so that we need only treat the renormalized spin waves of the system. We work effectively on the line of zero-fugacity renormalization-group fixed points with $0 \leq T \leq T_{KT}$. In the limit $V_0 \to \infty$ the field, coarse grained beyond the pair scale, has unit magnitude. We change to the phase variables $\vec{\phi} = e^{i\theta}$ and the energy-functional takes the form

$$H = \frac{\rho_s}{2} \int (\nabla \theta)^2 d^2\mathbf{x}, \qquad (3)$$

where ρ_s is the coarse-grained spin-wave stiffness of the system [4]. The equation of motion (1) simplifies to

$$\dot{\theta}_\mathbf{k} = -\rho_s \Gamma k^2 \theta_\mathbf{k} + \xi_\mathbf{k}, \qquad (4)$$

where we only keep the component of the thermal noise locally orthogonal to the order parameter $\vec{\phi}$, with $\langle \xi_\mathbf{k}(t) \xi_{\mathbf{k}'}(t') \rangle = 2\Gamma k_B T \delta_{\mathbf{k}, -\mathbf{k}'} \delta(t - t')$. (We will adsorb Γ

and ρ_s into the time scale, making $[t]$ dimensionally equivalent to $[l]^2$ for the rest of the paper, except when we discuss quenches with general temperature history.) We have ignored the 2π periodicity of θ in Eq. (4) because our system has no vortices after coarse graining so that the phase can be taken to be continuous everywhere.

The solution to the equation of motion (4) is

$$\theta_{\mathbf{k}}(t) = \theta_{\mathbf{k}}(0)e^{-k^2 t} + \int_0^t d\bar{t}\, e^{-k^2(t-\bar{t})}\xi_{\mathbf{k}}(\bar{t}), \qquad (5)$$

where the time $t \geq 0$ is measured from the time of the quench. Since we start from an equilibrated state at or below T_{KT}, the initial phases are determined by the spin-wave Hamiltonian (3). The Fourier transformed phases are Gaussian distributed with a probability distribution

$$P[\{\theta_{\mathbf{k}}(0)\}] \propto \exp\left\{ -\sum_k \frac{k^2}{4\pi\eta_i}\theta_{\mathbf{k}}(0)\theta_{-\mathbf{k}}(0)\right\}. \qquad (6)$$

We use η_i and η_f to describe the initial and final quench states, respectively, of our system, with $\eta(T) = k_B T/2\pi\rho_s(T)$. They describe the decay of equilibrium correlations and so are directly measurable in experiments. The "temperature" T always indicates the combination of system parameters (temperature, pressure, composition, etc.) that determine ρ_s and η.

The phase-phase correlations at general times after a quench at $t=0$ from a temperature T_i to a temperature T_f, both at or below T_{KT} [10], are then straightforward to calculate from (5)

$$\langle \theta_{\mathbf{k}}(t)\theta_{-\mathbf{k}}(t')\rangle = \frac{2\pi}{k^2}[\eta_f e^{-k^2|t'-t|} + (\eta_i - \eta_f)e^{-k^2(t+t')}]. \qquad (7)$$

In particular, the initial correlations are given by $\langle \theta_{\mathbf{k}}(0)\theta_{-\mathbf{k}}(0)\rangle = 2\pi\eta_i/k^2$. The phase-difference correlations then follow,

$$B(r,t,t') \equiv \langle[\theta(\mathbf{x},t) - \theta(\mathbf{x}+\mathbf{r},t')]^2\rangle$$
$$= \int \frac{d^2\mathbf{k}}{(2\pi)^2}[\langle \theta_{\mathbf{k}}(t)\theta_{-\mathbf{k}}(t)\rangle + \langle \theta_{\mathbf{k}}(t')\theta_{-\mathbf{k}}(t')\rangle$$
$$- 2\cos(\mathbf{k}\cdot\mathbf{r})\langle \theta_{\mathbf{k}}(t)\theta_{-\mathbf{k}}(t')\rangle]$$
$$= B_{eq}(r,t,t') + B_{neq}(r,t,t'). \qquad (8)$$

B_{eq} and B_{neq} are the equilibrium and nonequilibrium correlations at the final temperature, given by the terms proportional to η_f and $\eta_i - \eta_f$, respectively, in (7):

$$B_{eq}(r,t,t') = \eta_f\{\gamma + \ln(r^2/4a_0^2) + E_1[r^2/4(a_0^2 + |t-t'|)]\}, \qquad (9)$$

and

$$B_{neq}(r,t,t') = (\eta_i - \eta_f)\left\{\gamma + \ln\left(\frac{r^2}{4\sqrt{(a_0^2 + 2t)(a_0^2 + 2t')}}\right) + E_1[r^2/4(a_0^2 + t + t')]\right\}, \qquad (10)$$

where $E_1(x) \equiv \int_x^\infty dy\, e^{-y}/y$ for $x > 0$ and $\gamma \approx 0.577$ is Euler's constant. [We have used a soft ultraviolet cutoff, through a factor of $\exp(-a_0^2 k^2)$ in the integrand of each $\mathbf{k}$ integral, where a_0 is of the order of the lattice spacing.] Both B_{eq} and B_{neq} are manifestly symmetric under interchange of t and t'. B_{eq} only depends on the magnitude of the time difference $|t-t'|$ as expected for an equilibrium correlation. Conversely, B_{neq} has a scaling form at late times,

$$B_{neq}(r,t,t') = F(r/\sqrt{t}, r/\sqrt{t'}), \qquad t,t' \gg a_0^2, \qquad (11)$$

where $F(x)$ is a time-independent scaling function.

Order-parameter correlations follow directly from the phase correlations since the phase variables are Gaussian distributed at all times—due to the linear evolution equation (5) and the Gaussian nature of the noise and the initial conditions. The general two-point two-time correlation function is

$$C(r,t,t') \equiv \langle \vec{\phi}(\mathbf{x},t)\cdot\vec{\phi}(\mathbf{x}+\mathbf{r},t')\rangle,$$
$$= \langle\cos([\theta(\mathbf{x},t) - \theta(\mathbf{x}+\mathbf{r},t')])\rangle,$$
$$= \exp\{-B(r,t,t')/2\}$$
$$= C_{eq}(r,|t-t'|)C_{neq}(r,t,t'), \qquad (12)$$

where $C_{eq}(r,|t-t'|) \equiv \exp\{-B_{eq}(r,t,t')/2\}$ and $C_{neq}(r,t,t') \equiv \exp\{-B_{neq}(r,t,t')/2\}$. We see that $C(r,t,t')$ has a product scaling form, with a growing length scale of $L \propto t^{1/2}$ characterizing the nonequilibrium factor C_{neq} through Eq. (11). For quenches to $T_f > 0$, the equilibrium factor C_{eq} has a nontrivial form equal to the equilibrium correlation function of the critical point at the final temperature. This is a generalization of the scaling expected for a quench to within an ordered phase, dominated by a $T=0$ fixed point, where $C_{eq}(r) = \langle|\vec{\phi}|\rangle^2$. We do not expect the product form seen in Eq. (12) to hold for general $O(n)$ systems for quenches to critical points; the product form holds for this XY system due to the Gaussian distribution of the phase variables.

It is interesting to contrast these scaling results to the scaling prediction $L \sim (t/\ln t)^{1/2}$ [2], for quenches with free vortices, observed in simulations [5] (note also [11]). Quenches from below T_{KT} are consistent with previous energy-scaling predictions [2] which are based on the observed late-time defect structure for quenches to $T=0$. For nonconserved quenches without topological defects, a growth law $L(t) \sim t^{1/2}$ is predicted for systems which scale [2]—in agreement with the results of this paper. For quenches to $T > 0$, the energy-scaling approach does not directly apply. However, it is reassuring to note that scaling and the same growth law is observed in the nonequilibrium correlations C_{neq}.

We determine the asymptotic correlations by using the asymptotics of $E_1(x)$:

$$E_1(x) \sim \begin{cases} -\gamma - \ln x, & x \ll 1 \\ e^{-x}/x, & x \gg 1. \end{cases} \qquad (13)$$

These determine the asymptotic equilibrium correlations

$$C_{eq}(r,0) \sim (r/a_0)^{-\eta_f}, \qquad r \gg a_0 \qquad (14)$$

which reproduce the standard result [4]. The full equal-time correlations after the quench have the asymptotic behavior

$$C(r,t,t) \simeq \begin{cases} (r/a_0)^{-\eta_i}(\sqrt{t}/a_0)^{\eta_i - \eta_f}, & r^2/t \gg 1 \\ (r/a_0)^{-\eta_f}, & r^2/t \ll 1 \end{cases} \qquad (15)$$

where $r, \sqrt{t} \gg a_0$. They have the same spatial dependence as the equilibrium correlations (with the final temperature determining the correlations at short distances and the initial conditions determining them at long distances), but have an additional amplification factor at long scales. For $\eta_i = \eta_f$ we recover the equilibrium correlations (14), as expected.

The autocorrelation function is given by the $r=0$ correlations with initial conditions. From Eqs. (8)–(13),

$$A(t) \equiv C(0,t,0) \sim \left(\frac{t}{a_0^2}\right)^{-(\eta_i + \eta_f)/4}, \qquad (16)$$

where again we take $t \gg a_0^2$. Using $L \sim t^{1/2}$ and $A(t) \sim L^{-\bar{\lambda}}$ [6] we determine the exponent $\bar{\lambda} = (\eta_i + \eta_f)/2$ that describes the decay of autocorrelations after a quench. Interestingly, $\bar{\lambda}$ does not change if the quench is reversed: from η_f to η_i. For the decay of equilibrium autocorrelations, we set $\eta_f = \eta_i = \eta$ and find $\bar{\lambda}_{eq} = \eta$.

Bray et al. [9] have considered quenches from long-range correlated initial conditions to $T_f = 0$ ($\eta_f = 0$). They predict that if initial long-range correlations are described by $C(r,0) \sim r^{\sigma - d}$, and if $\sigma < \sigma_c$, then $C(r,t) \sim (L/r)^{d-\sigma}$ for $r \gg L$ and $A(t) \sim t^{(\sigma - d)/4}$ for large t. For quenches from a critical point, $\sigma = 2 - \eta$. Our results for quenches to $T=0$ agree (with $d=2$): from Eq. (15) we have $C \sim (L/r)^{\eta_i}$ with $L \sim t^{1/2}$, while from Eq. (16) we have $A(t) \sim t^{-\eta_i/4}$. The initial correlations are relevant for quenches from all temperatures at or below T_{KT}, so that $\sigma_c \leq 2 - \eta(T_{KT}) = 7/4$. Because $\bar{\lambda}_{SR}$, the value for short-range correlated initial conditions, is never less than $\bar{\lambda}$ for long-range correlated initial conditions [9], we have $\bar{\lambda}_{SR} \geq \bar{\lambda}(T_{KT}) = 1/8$ for a quench to $T_f = 0$. This lower bound is much smaller than the values measured by Pargellis et al. [8]. Theoretical treatments of quenches to critical points [12] have previously only treated the case of a quench with uncorrelated initial conditions, where $\bar{\lambda}$ is independent of the details of the initial conditions. The methods of reference [9] can be extended to general systems, in d dimensions, with a quench to a general critical point T_f [characterized by an equilibrium correlation function $C(r) \sim r^{-(d-2+\eta_f)}$], from a state with power-law spatial correlations (in the same order-parameter field) decaying as $r^{-(d-2+\eta_i)}$. We find $\bar{\lambda} = d-2 + (\eta_i + \eta_f)/2$ [13], provided that the long-range correlations in the initial state are relevant, which requires that the exponent $\bar{\lambda}_{SR}$ for a quench to T_f from initial conditions with short-range correlations satisfy $\bar{\lambda}_{SR} < d + (\eta_f - \eta_i)/2$. For quenches between two critical points in the 2D XY model, our result $\bar{\lambda} = (\eta_i + \eta_f)/2$ agrees

with the general result for $d=2$, and depends on both the initial and the final temperatures of the quench.

Arbitrary temperature histories of the quench can be treated in a similar manner to our discussion so far. We assume that the thermal bath has a well-defined time-dependent temperature $T = T(t)$, i.e., that microscopic time scales are much faster than the phase-ordering time scales. Then the renormalized spin-wave stiffness, $\rho_s(T)$, and the equilibrium decay exponent, $\eta(T)$, will both be time dependent through their temperature dependence. Equations (1)–(4) will be unchanged, while Eq. (5) will change to

$$\theta_{\mathbf{k}}(t) = \theta_{\mathbf{k}}(0)e^{-k^2 p(t)} + \int_0^t d\bar{t}\, e^{-k^2[p(t) - p(\bar{t})]}\xi_{\mathbf{k}}(\bar{t}), \qquad (17)$$

where $p(t) \equiv \int_0^t \rho_s(\bar{t})d\bar{t}$. This leads to the phase correlations

$$\langle \theta_{\mathbf{k}}(t)\theta_{-\mathbf{k}}(t')\rangle = \frac{2\pi\eta_i}{k^2} e^{-k^2[p(t) + p(t')]}$$

$$+ 2k_B \int_0^{\min(t,t')} d\bar{t}\, e^{-k^2[p(t) + p(t') - 2p(\bar{t})]} T(\bar{t}). \qquad (18)$$

This can be used in Eqs. (8) and (12) to determine correlations under an arbitrary temperature history. It is straightforward to show that temperature changes before a time t_M do not affect correlations with $t, t' \gg t_M$ or autocorrelations $A(t)$ for $t \gg t_M$. This is best illustrated by considering autocorrelations in the low-fugacity limit, where ρ_s is temperature independent. With some work, we have $B(0,0,t) = (\eta_i/2)\ln(t/a_0^2) + \int_0^t d\bar{t}\, \eta(\bar{t})/(a_0^2 + 2t - 2\bar{t})$. [We have adsorbed the constant ρ_s into $\eta(t)$.] If we restrict the time dependence of T to times before $t_M \ll t$, then $B(0,0,t) = \ln(t/a_0^2)(\eta_i + \eta_f)/2 + O(t_M/t)$ and we recover our previous result. The same approach demonstrates that late-time correlations and autocorrelations are insensitive to the temperature history before a time $t_M \ll t$. Exact correlations for simple quench histories can easily be calculated, and may be useful for comparing to experiments, but do not appear qualitatively different than instantaneous quenches.

The ease of calculation of this model is fortuitous. This is because, in part, for vector systems, the gradient term in Eq. (2) dominates over the potential term [2]. Since the potential term is not needed to set a core scale for singular defects (such as free vortices), the hard-spin limit may be taken without complications. The 2D XY model is special below T_{KT} because the vortices are tightly bound and only serve to renormalize the spin-wave stiffness ρ_s of the effective hard-spin Hamiltonian. The resulting Gaussian nature of the phase variables greatly simplifies the analysis. (Note that the hard-spin limit for conserved "model B" dynamics [3] leads to a much more complicated evolution equation than (4), and the phases will not be Gaussian distributed.) Of course, our results only apply for distances that are large with respect to the vortex pair size in the two equilibrium phases at T_i and T_f [14].

The specially prepared nematic system of Pargellis et al. [8], developed to exhibit 2D XY behavior, should exhibit the behavior described in this paper. The experimental procedure

will be easier since late time correlations and autocorrelations do not depend on the early stages of the quench. (Experimental analysis will not be able to rely, however, on the characteristic schlieren patterns of free vortices, which will be absent.)

We have calculated correlations for quenches in the 2D *XY* model between any two phases at or below the Kosterlitz-Thouless temperature. The nonequilibrium part of the correlations scales with a characteristic length scale $L(t) \sim t^{1/2}$. This growth law differs by a logarithmic factor from the growth laws expected for quenches involving free vortices. The autocorrelation decay exponent depends on both the initial and the final state of the quench, $\bar{\lambda} = (\eta_i + \eta_f)/2$. The asymptotic autocorrelations and equal-time correlations do not depend on the early temperature history of the quench, but only on the initial conditions (through η_i) and on the temperature at late times (through η_f).

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[10] In terms of the exponents describing the equilibrium correlations, we consider quenches between any two states with $\eta \leqslant 1/4$, the value at T_{KT} [4].

[11] Nontrivial phase-ordering scalar systems always form domains, and most dynamically scaling systems with more than two components have the same growth law in systems with or without topological defects. However, for the nonconserved 2D *XY* model and the conserved $d > 2$ *XY* models different growth laws are expected for scaling systems with and without topological defects [2], and so these may be candidates for scaling violations or for large corrections to scaling. This may be related to possible scaling violations observed in nonconserved 2D *XY* models [R. E. Blundell and A. J. Bray, Phys. Rev. E **49**, 4925 (1994)], and in models of nematic liquid crystals [M. Zapotocky, P. M. Goldbart, and N. Goldenfeld, Phys. Rev. E **51**, 1216 (1995)], quenched from above T_{KT}.

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[14] At distances comparable to the vortex pair size the bound vortices will affect the correlations. In particular, the Fourier transformed correlations $S(k,t)$ will have a weak power-law Porod tail k^{-4} with amplitude proportional to the vortex pair density for $k \to \infty$.