Unwinding Scaling Violations in Phase Ordering

A. D. Rutenberg and A. J. Bray

Theoretical Physics Group, Department of Physics and Astronomy, The University of Manchester, M13 9PL, United Kingdom (Received 18 October 1994)

The one-dimensional O(2) model is the simplest example of a system with topological textures. The model exhibits anomalous ordering dynamics due to the appearance of *two* characteristic length scales: the phase *coherence* length $L \sim t^{1/z}$ and the phase *winding* length $L_w \sim L^x$. We derive the scaling law $z = 2 + \mu \chi$, where $\mu = 0$ ($\mu = 2$) for nonconserved (conserved) dynamics and $\chi = 1/2$ for uncorrelated initial orientations. From hard-spin equations of motion, we consider the evolution of the topological defect density and recover a simple scaling description.

PACS numbers: 64.60.Cn, 05.70.Ln, 64.60.My

The scaling hypothesis has played an important role in our understanding of the late-stage ordering dynamics of systems quenched from a homogeneous disordered phase into an ordered phase region with a broken symmetry [1]. According to this hypothesis, the order parameter morphology at late times after the quench is statistically independent of time if all lengths are rescaled by a single characteristic length scale L(t). This implies that the pair correlation function C(r,t) of the order parameter should depend on its arguments only through the ratio r/L(t). Recently, we have shown [2] that a natural extension of the scaling hypothesis to two-time correlations, C(r,t,t') = f(r/L(t),r/L(t')), supplemented by an understanding of the short-distance [i.e., $r \ll L(t)$] structure that follows from any singular topological defects seeded by the quench [3], determines the late-time growth law of L(t). Any departure from these growth laws implies a breakdown of the single-length scaling.

Given the importance of the scaling phenomenology, it is important to look for exceptions to single-length scaling, and to try to understand them within a broader scaling framework. There is evidence that some systems with nonsingular topological textures may violate conventional single-length scaling. Textures have a spatial extent, which can, in principle, introduce a new characteristic length scale. The O(n) model for an n-component vector field in spatial dimension d=n-1 provides a class of models with topological textures. Indeed, the O(3) model in d=2 seems to have at least one of its characteristic scales growing as $t^{1/3}$ for nonconserved dynamics [4,5], which contrasts with the anticipated $t^{1/2}$ growth for this system if scaling holds [2,5].

The O(2) model (or "XY model") in spatial dimension d=1 is the simplest system with topological textures. We show through the time-derivative correlations, $T(r,t) = \partial_t \partial_{t'}|_{t=t'}C(r,t,t')$, that single-length scaling fails in this system, for both conserved and nonconserved dynamics. The nonconserved case is exactly soluble [6,7]: One finds that C(r,t) scales with a length scale $t^{1/4}$, different from the $t^{1/2}$ scaling predicted from the scaling hypothesis [2], and T(r,t) scales with the same length scale but with an anomalous time-dependent prefactor.

We show, within a general framework, that this discrepancy is due to the existence of *two* characteristic length scales, the "phase coherence length" $L \sim t^{1/2}$, and the "phase winding length," $L_w \sim t^{1/4}$. Since L_w is the typical length scale over which the phase changes by order unity (see Fig. 1), it provides the characteristic scale for the pair correlation function. The phase coherence length L drives the dynamics and enters into the two-time correlation functions, such as T(r,t).

In contrast to the nonconserved model, the conserved model has not previously been addressed except by computer simulations. The same concepts are relevant to this case also, however, and by means of a simple scaling argument we find $L \sim t^{1/3}$ and $L_w \sim t^{1/6}$, the latter in agreement with recent simulations [7,8].

The issue of scaling in these systems is clarified by showing that the phase-difference correlation function G(r,t) (11), rather than the order parameter correlation function, exhibits a generalized form of single-length scaling with characteristic length L. The topological charge

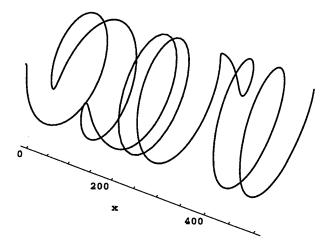


FIG. 1. A section of a system from a simulation using nonconserved dynamics. Distance along the system is shown by the scale, and the unit-magnitude order parameter is shown in the orthogonal plane. The windings of $\pm 2\pi$ (textures or antitextures) of scale L_w and the clusters of monotonic winding of a larger scale L are evident.

density, proportional to the phase gradient, provides an equivalent description that exemplifies the simple scaling description.

The key elements of this paper are (i) the development of hard-spin equations of motion for conserved dynamics, (ii) the simplification of the equations of motion at late times using the separation of the length scales L and L_w , (iii) the scaling relations for the length scales, and the consequent forms for spin-spin correlations C(r,t) and T(r,t), and (iv) the unifying scaling description in terms of the topological charge density.

Figure 1 shows a typical configuration generated by a computer simulation with nonconserved dynamics. The configuration consists of sections of typical length L where the order parameter winds in a given sense, alternating with antiwinding sections. The winding length L_w is the typical distance between successive windings of 2π in the phase. Since each complete winding (antiwinding) represents a topological texture (antitexture) in this system, L_w is the characteristic texture size. During the phase ordering process, because isolated textures expand [9], textures unwind by annihilating with adjacent antitextures at the boundaries between regions of positive and negative winding.

We begin with a heuristic argument relating L and L_w . Consider a region of length l. If the phase angles in the initial condition have only short-range correlations, with correlation length ξ_0 , then the initial net winding over the length l is of order $(l/\xi_0)^{1/2}$. Because the total winding is a topological invariant, the net winding on scales much larger than the phase coherence length $l \gg L$ will be unchanged. At later times, the length l contains of order l/L sections, each winding in a given sense, with of order L/L_w windings per section. The net winding is therefore $(l/\xi_0)^{1/2} \sim (L/L_w)(l/L)^{1/2}$, giving $L_w \sim (L\xi_0)^{1/2}$. (We assume here that the fluctuations in the total winding per section are comparable with the mean winding.) This indicates that two time-dependent lengths characterize the system.

We now present an explicit calculation that verifies our heuristic argument and gives the growth laws for L and L_w . It is convenient to formulate the problem in terms of the U(1) model for a complex scalar field $\phi = \rho \exp(i\theta)$. We take the conventional Ginzburg-Landau free-energy functional

$$F[\phi] = \int dx [(\partial_x \phi)(\partial_x \phi^*) + (g/2)(1 - \phi \phi^*)^2]. \quad (1)$$

The purely dissipative equation of motion is

$$\partial_t \phi = -(-\partial_x^2)^{\mu/2} \, \delta F / \delta \phi^*, \tag{2}$$

where $\mu=0$ and 2 for nonconserved and conserved dynamics, respectively. It is mathematically convenient to take the limit $g\to\infty$, which imposes the constraint $|\phi|=1$, corresponding to a nonlinear sigma model or "hard-spin" description. This limit is taken by writing $\phi=\exp(i\theta-\beta/g)$ in (2), expanding in β/g , and re-

taining only terms of order unity. [This method can be quite generally applied to conserved vector systems by taking $\dot{\phi} = \exp(-\beta/g)\dot{\phi}$, where $|\dot{\phi}| = 1$.] For the 1D XY model, we obtain

$$i\dot{\theta}\exp(i\theta) = (-\partial_x^2)^{\mu/2} [i\theta'' - (\theta')^2 + 2\beta] \exp(i\theta), \quad (3)$$

where dots and primes indicate derivatives with respect to t and x.

Consider first the nonconserved case, $\mu = 0$. Equating real and imaginary parts in (3) gives

$$\dot{\theta} = \theta'', \tag{4}$$

$$\beta = (\theta')^2/2. \tag{5}$$

Thus the phase equation (4) decouples from the amplitude equation (5), and the amplitude is slaved to the phase.

For the conserved case, $\mu=2$, the same treatment yields coupled equations for θ and β . Motivated by Eq. (5), we put $\beta=(\theta')^2/2+\gamma$, where we anticipate that γ will be negligible at late times. The resulting equations are

$$\dot{\theta} = (\theta')^2 \theta'' - \theta'''' - 2\gamma \theta'' - 4\gamma' \theta', \tag{6}$$

$$2\gamma'' = 2(\theta')^2 \gamma + 2\theta' \theta''' + (\theta'')^2. \tag{7}$$

It is easy to show explicitly that these equations conserve the order parameter, i.e., $\partial_t \int dx \exp(i\theta) = 0$.

An equivalent approach to deriving the hard-spin equations (4)–(7) starts from (1) with g=0 and the condition $|\phi|=1$ imposed through a Lagrange multiplier. This leads directly to (3), 2β being the Lagrange multiplier.

As a consequence of the two length scales in the problem, the first term on the right of (6) dominates at late times, so that the phase equation (6) again decouples from the amplitude equation (7) at late times. The key point is that while the typical size of θ' is given by $\theta' \sim 1/L_w$, the spatial variation of θ' occurs on the longer scale L (see Fig. 2). Thus each higher derivative generates an extra factor of 1/L, giving $\theta'' \sim 1/LL_w$, $\theta''' \sim 1/L^2L_w$, etc. Thus on the right of (6) $\theta'''' \sim 1/L^3L_w$ is negligible compared to $(\theta')^2\theta'' \sim 1/LL_w^3$. Now look at Eq. (7). Demanding that $(\theta')^2\gamma \sim \theta'\theta''' \sim (\theta'')^2 \sim 1/L^2L_w^2$ gives $\gamma \sim 1/L^2$ (and on the left, $\gamma'' \sim 1/L^4$ is negligible). Putting this into (6), we find that the terms involving γ are both of order $1/L^3L_w$ and therefore negligible at late times. Thus the first term on the right of (6) dominates at late times, giving the simplified dynamics

$$\dot{\theta} = (\theta')^2 \theta''. \tag{8}$$

This equation is one of the central results of the paper, and represents a significant simplification of the original equation of motion. Although Eq. (8) no longer conserves the order parameter at all times, the omitted terms on the right of (6) are of relative order $L_w^2/L^2 \sim 1/L$, and the conservation is asymptotically recovered at late times.

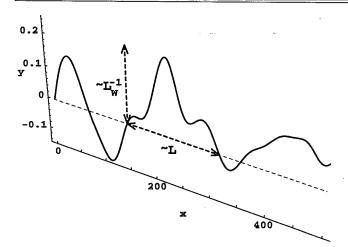


FIG. 2. The phase gradient $y \equiv \theta'$ vs distance is shown corresponding to the section of the system shown in Fig 1. The characteristic length scales are indicated: L is the average distance between zeros of θ' , while $2\pi/L_w$ is the characteristic magnitude of θ' .

The key step in deriving the growth exponents for L and L_w is to transform from the phase variable θ to the phase gradient $y = \theta'$. Note that $\rho(x) = y(x)/2\pi$ is just the local winding rate or the "topological charge density" at point x. Our basic assumption is that, whereas the order parameter representation sketched in Fig. 1 can never be made scale invariant due to the two different length scales, the same morphology in the y representation of Fig. 2 is scale invariant under a simultaneous rescaling of x by L and y by $1/L_w \sim 1/L^x$ (where we anticipate $\chi = 1/2$ from our heuristic argument). This is an important generalization of the standard dynamical scaling hypothesis, and is confirmed by exact calculation for nonconserved dynamics and by simulation for conserved dynamics [7].

For compactness, we combine (4) and (8) as the single equation $\dot{\theta} = (\theta'^2)^{\mu/2}\theta''$. In terms of y, this reads

$$\dot{y} = [(y^2)^{\mu/2} y']' \qquad (y \equiv \theta').$$
 (9)

Making the scale transformations $x \to bx$, $t \to b^z t$, $y \to b^{-x} y$ in (9), and demanding scale invariant behavior gives our main result,

$$z = 2 + \mu \chi. \tag{10}$$

(Although we have derived this result only for $\mu=0$ and $\mu=2$, the cases of greatest physical interest, we expect it to hold for general $\mu\geq 0$ [7].)

To determine the exponent χ , and to exemplify the scaling, it is convenient to introduce the squared phase difference correlation function

$$G(r,t) = \langle [\theta(x+r,t) - \theta(x,t)]^2 \rangle$$

= $L^{2(1-\chi)}g(r/L)$, (11)

where the scaling form follows from the scaling transformations above and from noting that phase differences scale as L^{1-x} . [Alternatively, we could work with the

phase gradient (or topological charge density) correlation function $H(r,t) = \langle y(x+r)y(x) \rangle = L^{-2\chi}h(r/L)$.]

The angular brackets in (11) represent an average over an ensemble of initial conditions. A natural choice of initial conditions is the Gaussian distribution

$$P[\theta(x,0)] \propto \exp\left\{-\sum_{k} \theta_{k}(0)\theta_{-k}(0)/2\sigma_{k}\right\}, \quad (12)$$

where $\theta_k(0)$ is the Fourier amplitude of $\theta(x,0)$. The pair correlation function for the order parameter at t=0 then takes the form

$$C(r,0) = \langle \phi(x+r,0)\phi^*(x,0)\rangle$$

$$= \exp\{-\langle [\theta(x+r,0)-\theta(x,0)]^2\rangle/2\}$$

$$= \exp\{-\sum_{k} \sigma_k (1-\cos kr)\}.$$
 (13)

Choosing $\sigma_k = 2/\xi_0 k^2$ yields $C(r,0) = \exp(-r/\xi_0)$, appropriate to a quench from a disordered phase with correlation length ξ_0 . This corresponds to a "random walk" of the initial phase angles, so that $G(r,0) = 2r/\xi_0$.

Now consider the dynamics. Since the topological charge is locally conserved, the development of phase coherence at scale L due to texture-antitexture annihilation does not affect the phase-difference correlation function at larger separations $r \gg L$, i.e., $G(r,t) \to 2r/\xi_0$ in this limit. Hence from Eq. (11), the scaling function $g(x) \sim x$ for $x \to \infty$, and since L must drop out in this limit we have

$$\chi = 1/2. \tag{14}$$

Putting this into (10) gives $z = 2 + \mu/2$, and so

$$L \sim t^{2/(4+\mu)},\tag{15}$$

$$L_w \sim L^{1/2} \sim t^{1/(4+\mu)}$$
. (16)

Previous studies of phase ordering systems have usually concentrated on the pair correlation function C(r,t), and its Fourier transform, the structure factor S(k,t). In the present context, the phase difference correlation function G(r,t) is more appropriate, as it reveals the full scaling structure (11). The scaling properties of C(r,t) can, however, be inferred. The usual pair correlation function is given by

$$C(r,t) = \langle \exp\{i[\theta(x+r,t) - \theta(x,t)]\}\rangle$$

= $\langle \exp\{i(ry+r^2y'/2+r^3y''/6+\cdots)\}\rangle$, (17)

where the second line follows from the Taylor series expansion of $\theta(x+r,t)$. In the late-time limit $r \to \infty$, $L_w \to \infty$, with r/L_w fixed, only the leading term in the expansion survives, because $ry \sim r/L_w$ is of order unity, while $r^2y' \sim r^2/LL_w$ is of order $L_w/L \ll 1$, and the higher terms are smaller still. This limit probes correlations on the scale L_w , since L_w^{-1} sets the scale of $y \equiv \theta'$, so that

$$C(r,t) = \langle \exp(iry) \rangle$$

= $f(r/L_w)$, (18)

where $L_w \sim t^{1/4}$ for $\mu = 0$ and $t^{1/6}$ for $\mu = 2$. Because the structure factor S(k, t) is the spatial Fourier transform of C(r,t), from (18) we see that S(k,t) = P(k,t), where P(y,t) is the single-point probability distribution for y. For $\mu = 0$, the linear dynamics (4) combined with the Gaussian initial condition (13) ensures that the probability distribution, and hence S(k, t) and C(r, t) are Gaussian at all times. The exact solution of the model [6,7] confirms this feature, with the expected scale length $L_w \sim t^{1/4}$. For the conserved case, the conservation requires that S(k, t) vanish at k = 0, implying P(0, t) = 0 in the scaling limit. Thus P(y,t) cannot be Gaussian in this case, but must have a double peaked structure. Indeed, numerical studies indicate [7] that P(y, t) is approximately described by the form $P(y,t) \sim L_w^3 y^2 \exp(-\text{const} \times y^2 L_w^2)$, and are consistent [7,8] with the result $L_w \sim t^{1/6}$ derived above.

Time-derivative correlations probe the scaling properties of the full two-time correlations C(r,t,t'). In the same limit $r \to \infty$, $L_w \to \infty$, with r/L_w fixed, we have $T(r,t) \equiv \partial_t \partial_{t'}|_{t=t'}C(r,t,t') = \langle \theta^2 \exp\{i[\theta(x+r,t)-\theta(x,t)]\}\rangle = \langle y'^2y^{2\mu}\exp(iry)\rangle$, where we have used Eqs. (4) and (8) for θ . For the nonconserved case, because the variables are Gaussian and $\langle yy'\rangle = \langle (y^2)'\rangle/2 = 0$, then $T(r,t) = \langle y'^2\rangle\langle \exp(iry)\rangle = \langle y'^2\rangle C(r,t)$. For the conserved case, the phase variables are not Gaussian, so T(r,t) is not simply proportional to C(r,t). In both cases, we use $y \sim L_w^{-1}$ and $y' \sim (LL_w)^{-1}$ and the growth laws of Eqs. (15) and (16) to determine

$$T(r,t) = t^{-2(\mu+3)/(\mu+4)} \tilde{f}(r/L_w), \qquad (19)$$

which breaks dynamical scaling because the time-dependent amplitude is not proportional to t^{-2} [2]. Because the phase dynamics involves spatial gradients of y, the second length scale L is introduced and the dynamical scaling is broken.

These results can be generalized to a broader class of correlated initial conditions which includes a conventional scaling solution. If we take $\sigma_k \sim k^{-\alpha}$ in (13), we obtain $G(r,0) \sim r^{\alpha-1}$, provided $1 < \alpha < 3$. The requirement due to local phase conservation that this form be recovered from the general scaling form (11) when $r \gg L$ fixes

$$\chi = (3 - \alpha)/2, \tag{20}$$

$$z = 2 + \mu(3 - \alpha)/2,$$
 (21)

where we have applied Eq. (10). For $\mu=0$ we still have z=2 with $L\sim t^{1/2}$ and $L_w\sim t^{(3-\alpha)/4}$, but for $\mu=2$ we obtain $z=5-\alpha$, giving $L\sim t^{1/(5-\alpha)}$ and $L_w\sim L^{(3-\alpha)/2(5-\alpha)}$. For $\alpha=1$, we obtain $G(r,0)\sim \ln r$, implying a power-law decay of C(r,0). Simple scaling is recovered in the limit $\alpha\to 1$, since $\chi\to 1$ implies that L_w and L both grow in the same way, with characteristic scale $L\sim t^{1/2}$ for $\mu=0$, and $L\sim t^{1/4}$ for $\mu=2$. These growth laws are just what we expect for a one-dimensional O(2) system with simple scaling [2].

The essence of the "energy scaling" approach that determines the growth laws for single-length scaling

[2] can be used for an alternative derivation of the central result (10). In the hard-spin limit, the free-energy functional (1) becomes $F[\theta] = \int dx \, \theta'^2$. The energy density is therefore $\epsilon = \langle \theta'^2 \rangle \sim L_w^{-2} \sim L^{-2\chi}$. This gives the energy density dissipation rate as

$$\dot{\epsilon} \sim -\dot{L}L^{-(2\chi+1)}.\tag{22}$$

However, $\dot{\epsilon}$ may be independently estimated via

$$\begin{split} \dot{\epsilon} &= \langle (\delta F/\delta \theta) \dot{\theta} \rangle \\ &\sim -\langle \theta''^2 (\theta'^2)^{\mu/2} \rangle \sim -L_w^{-(2+\mu)} L^{-2} \sim -L^{-[2+\chi(2+\mu)]}. \end{split}$$

Equating these two estimates gives $L \sim t^{1/(2+\mu\chi)}$.

To summarize, we have shown that the ordering dynamics of the O(2) model in d = 1 involves two characteristic length scales: $L_w \sim t^{1/(4+\mu)}$ which acts as the scaling length for the order parameter correlation functions, though T(r,t) and, by implication, C(r,t,t') do not satisfy standard dynamical scaling, and $L \sim t^{2/(4+\mu)}$ which is the scaling length for correlations of the phase difference (or phase gradient). Working with the phase gradient, which is proportional to the topological charge density for this system, is necessary to provide a unifying framework. It is only by considering correlations of the phase differences that a simpler scaling description emerges. To what extent do scaling violations, and/or a simplified description in terms of the topological charge density, occur in higher-dimensional texture systems? Numerical simulations on the nonconserved 2D O(3) model indicate the existence of three different growing length scales, roughly corresponding to typical texture size, texture-texture separation, and texture-antitexture separation [5,10]. As yet, however, no simplifying description analogous to that presented here has been developed.

We thank T. Blum, W. Zakrzewski, and M. Zapotocky for discussions, and the Isaac Newton Institute, Cambridge, where this work was completed, for hospitality.

- [1] H. Furukawa, Adv. Phys. 34, 703 (1985); A. J. Bray, *ibid.* 43, 357 (1994).
- [2] A. J. Bray and A. D. Rutenberg, Phys. Rev. E 49, R27 (1994); A. D. Rutenberg and A. J. Bray, *ibid.* 51, 1641 (1995).
- [3] N.D. Mermin, Rev. Mod. Phys. 51, 591 (1979).
- [4] A. J. Bray and K. Humayun, J. Phys. A 23, 5897 (1990).
- [5] A.D. Rutenberg, Phys. Rev. E 51, 2715 (1995).
- [6] T. J. Newman, A. J. Bray, and M. A. Moore, Phys. Rev. B 42, 4514 (1990).
- [7] A.D. Rutenberg, A.J. Bray, and M. Kay (unpublished).
- [8] M. Mondello and N. Goldenfeld, Phys. Rev. E 47, 2384 (1993); M. Rao and A. Chakrabarti, *ibid.* 49, 3727 (1994).
- [9] G. H. Derrick, J. Math. Phys. 5, 1252 (1964).
- [10] For the 1D XY model, the first two of these lengths are equal.