

ARTICLES

Corrections to scaling in the phase-ordering dynamics of a vector order parameter

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Corrections to scaling, associated with deviations of the order parameter from the scaling morphology in the initial state, are studied for systems with $O(n)$ symmetry at zero temperature in phase-ordering kinetics. Including corrections to scaling, the equal time pair correlation function has the form $C(r,t)=f_0(r/L)+L^{-\omega}f_1(r/L)+\dots$, where L is the coarsening length scale. The correction-to-scaling exponent ω and the correction-to-scaling function $f_1(x)$ are calculated for both nonconserved and conserved order parameter systems using the approximate Gaussian closure theory of Mazenko. In general ω is a nontrivial exponent which depends on both the dimensionality d of the system and the number of components n of the order parameter. Corrections to scaling are also calculated for the nonconserved one-dimensional XY model, where an exact solution is possible. [S1063-651X(99)11308-4]

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I. INTRODUCTION

The dynamics of a system undergoing phase ordering following a quench from the high temperature (disordered) phase to the ordered phase is of great interest [1]. The kinetics of systems with $O(n)$ symmetry subject to “model A” dynamics [2] (i.e., systems with nonconserved order parameter) and “model B” dynamics [2] (systems with conserved order parameter) have been previously studied [3,4] within a Gaussian closure theory originally developed by Mazenko [5,6] following the seminal work of Ohta, Jasnow, and Kawasaki (OJK) [7]. In previous work [8] we have computed the form of the corrections to the scaling limit, and the correction-to-scaling exponent, for a number of systems with nonconserved order parameter. These include some exactly soluble models, and the model A dynamics of a scalar field within the Mazenko theory.

In the present work we turn our attention to systems with a vector order parameter, both nonconserved and conserved. The corrections to scaling for systems with continuous symmetry will be calculated using the Mazenko theory. It should be mentioned that this approach has been shown to be more successful, at a quantitative level, in systems with nonconserved order parameter than those with conserved order parameter [9]. Nevertheless, the results obtained in the conserved case are in qualitative agreement with those obtained in simulations. Furthermore, the Mazenko approach seems the only available method to probe the questions of corrections to scaling addressed here. In particular, we found that, for nonconserved scalar fields, the correction-to-scaling exponent ω is predicted by this approach to have a nontrivial value. We will show that this same feature is present for the vector fields, with and without conservation.

It is well established [1] that at late times most phase-ordering systems approach a scaling regime, where the equal-time pair correlation function $C(r,t)\equiv\langle\vec{\phi}(\mathbf{x}+\mathbf{r},t)\cdot\vec{\phi}(\mathbf{x},t)\rangle$ takes the form $C(r,t)=f[r/L(t)]$. The charac-

teristic length scale $L(t)$ grows with time as $L(t)\sim t^a$, where a is the growth exponent which depends on the nature of the dynamics and the symmetry of the order parameter. In particular, $a=1/2$ for nonconserved order parameter systems, while $a=1/3$ for systems with conserved scalar order parameter and $a=1/4$ for systems with conserved vector order parameter (with logarithmic corrections for $n=2$, $d>2$ [10]). In previous work [8] we studied how scaling is approached in nonconserved order parameter models such as the one-dimensional (1D) Ising model with Glauber dynamics, the n -vector model with $n=\infty$, the approximate OJK theory and the Mazenko theory for scalar fields. In all these cases ω was found to be trivial ($\omega=4$) except the last, for which ω was found to be non-trivial and dimensionality dependent. The relevance of corrections to scaling lies in interpreting experimental and simulation results, where it is advantageous to know how the scaling limit is approached. Corrections to scaling in systems with finite $n>1$ in $d=3$ and $d=2$ were not considered in [8]. The main objective in this article is to study systems with $n\geq 2$.

This article is devoted to the study of the corrections to scaling for systems with $O(n)$ symmetry in phase-ordering dynamics. The leading corrections to scaling enter the correlation function in the form

$$C(r,t)=f_0(r/L)+L^{-\omega}f_1(r/L), \quad (1)$$

where $f_0(x)$ is the “scaling function” and $f_1(x)$ the “correction-to-scaling function.” The quantity which unites theory, computer simulation and experiment is the structure factor $S(k,t)=L^d g_0(y)+L^{d-\omega} g_1(y)$, where $g_0(y)$ and $g_1(y)$ are the d -dimensional Fourier transforms of $f_0(x)$ and $f_1(x)$ respectively, and $y=kL$. Coniglio and Zannetti [11] solved the conserved $O(n)$ model for $n=\infty$ exactly, and found that no simple scaling exists. Instead a “multiscaling” behavior was obtained, raising the question of whether simple scaling exists in conserved order parameter systems

with $n > 1$ generally (or even for conserved scalar fields). However, it was later shown by Bray and Humayun [12], analytically within the Mazenko theory, that scaling does exist for large but finite n . Attempts to find multiscaling behavior in simulation data for conserved scalar fields [13], or the conserved XY model in two [14] or three [15] dimensions were not successful. It is now generally believed that scaling is recovered asymptotically in time in the conserved $O(n)$ model, for all finite n , though multiscaling may be observable in the preasymptotic regime [16].

There are other sources of corrections to scaling apart from the one considered in this paper. In phase-ordering systems there is, in addition to the time-dependent coarsening scale $L(t)$, a second characteristic length scale, the ‘‘defect core size’’ ξ , in systems with topological defects. The corrections to scaling associated with nonzero defect core size (where ξ is the domain wall thickness in scalar systems) are expected to enter as a power of ξ/L . Here we are interested primarily in the corrections to scaling associated with non-scaling initial conditions. We therefore suppress the contributions associated with nonzero core size ξ by taking the ‘‘hard-spin’’ limit, i.e., working with an order-parameter field whose length is everywhere unity, $\vec{\phi}^2 = 1$, which forces $\xi = 0$ (though in the Mazenko theory this limit will be taken at the end). Also thermal fluctuations at $T > 0$ may give rise to significant corrections to scaling for systems quenched to a nonzero final temperature T [17] (where $0 < T < T_c$, with T_c the critical temperature) as has been shown explicitly in the nonconserved $O(n)$ model with $n \rightarrow \infty$ [18]. However, we will only be studying systems quenched to $T = 0$. Although corrections to scaling due to thermal fluctuations and nonzero ξ are important we will not consider them further in this paper.

The outline of the paper is as follows. In the following section the approximate Mazenko theory is discussed and some general concepts are introduced. Section III deals with nonconserved order parameter systems. In Sec. IV, corrections to scaling for the nonconserved 1D XY model will be studied. Systems with conserved order parameter are considered in Sec. V. Section VI concludes with a summary and discussion.

II. MAZENKO THEORY

A ‘‘Gaussian closure’’ theory, building on the earlier work of Ohta, Jasnow, and Kawasaki [7] has been developed by Mazenko [5]. This theory has been successfully applied to $O(n)$ models in the theory of phase-ordering dynamics [3,9]. The equation of motion for an order parameter $\vec{\phi}$ with continuous symmetry, for systems quenched to $T = 0$, is

$$\frac{\partial \vec{\phi}(1)}{\partial t_1} = (-\nabla_1^2)^p \left[\nabla_1^2 \vec{\phi}(1) - \frac{\partial V[\vec{\phi}(1)]}{\partial \vec{\phi}(1)} \right], \quad (2)$$

where $p = 1$ and $p = 0$ for conserved order parameter (model B) and nonconserved order parameter (model A) systems, respectively. In Eq. (2), $V(\vec{\phi})$ is a symmetric double-well potential for the scalar case, and a ‘‘wine bottle’’ potential with a degenerate continuum manifold for a vector order parameter. Compact notation has been used in which ‘‘1’’

represents the space-time point (\vec{x}_1, t_1) and ∇_1^2 means the Laplacian with respect to \vec{x}_1 . Multiplying Eq. (2) by $\vec{\phi}(2)$, averaging over initial conditions, and using the translational invariance of $C(12)$ gives (for $t_1 = t_2 = t$)

$$\frac{1}{2} \frac{\partial C(12)}{\partial t} = (-\nabla^2)^p \left[\nabla^2 C(12) - \left\langle \frac{\partial V[\vec{\phi}(1)]}{\partial \vec{\phi}(1)} \cdot \vec{\phi}(2) \right\rangle \right], \quad (3)$$

where now ∇^2 is the Laplacian with respect to $r = |\mathbf{x}_1 - \mathbf{x}_2|$ and $C(12) = \langle \vec{\phi}(1) \cdot \vec{\phi}(2) \rangle$. The angular brackets denote the average over the initial conditions. In order to evaluate the average of the last term in Eq. (3) one introduces an auxiliary field $\vec{m}(r, t)$ related to $\vec{\phi}$ by $\nabla_m^2 \vec{\phi} = 2\partial V(\vec{\phi})/\partial \vec{\phi}$, with boundary condition $\vec{\phi} \rightarrow \vec{m}/|\vec{m}|$ as $|\vec{m}| \rightarrow \infty$, and $\vec{\phi} = 0$ at $\vec{m} = 0$. Near a defect, the field $\vec{m}(\mathbf{r})$ is the position vector of the point \mathbf{r} in the plane normal to the defect. The assumption that \vec{m} is a Gaussian field enables the evaluation of the average of the last term on the right hand side of Eq. (3) giving [3]

$$\frac{1}{2} \frac{\partial C(12)}{\partial t} = (-\nabla^2)^p \left[\nabla^2 C(12) + \frac{1}{2S_0(1)} \gamma \frac{dC(12)}{d\gamma} \right], \quad (4)$$

where $S_0 = \langle m(1)^2 \rangle$ and

$$\gamma(12) = \langle m(1)m(2) \rangle / [\langle m(1)^2 \rangle \langle m(2)^2 \rangle]^{1/2}$$

is the normalized correlator of the field m (where m is one of the components of \vec{m}). An explicit expression which relates γ to $C(12)$ was given in [19]

$$C = \frac{n\gamma}{2\pi} \left[B\left(\frac{n+1}{2}, \frac{1}{2}\right) \right]^2 F\left(\frac{1}{2}, \frac{1}{2}; \frac{n+2}{2}; \gamma^2\right), \quad (5)$$

where $B(y, z) = \Gamma(y)\Gamma(z)/\Gamma(y+z)$ is the Beta function and $F(a, b; c; z)$ the hypergeometric function. Equations (4) and (5) provide closed form equations for $C(12)$. On substituting Eq. (5) in Eq. (4) one obtains an equation for γ which can in principle be solved numerically and substituted back into Eq. (5) to obtain the correlation function $C(12)$. We note at this point that in deriving the correlation function (5), the ‘‘hard-spin’’ limit $\phi = \vec{m}/|\vec{m}|$ was employed. Since this result holds far from defect cores, it will correctly describe the scaling limit where the defects are dilute. Here we are also using it to compute the corrections to scaling.

III. NONCONSERVED $O(N)$ MODEL

For a nonconserved system $p = 0$, and Eq. (4) is simply

$$\frac{1}{2} \frac{\partial C(12)}{\partial t} = \nabla^2 C(12) + \frac{1}{2S_0(1)} \gamma \frac{dC(12)}{d\gamma}. \quad (6)$$

For $n = 1$, using the properties of the hypergeometric function the last term on the right hand side of Eq. (6) can be written in terms of $C(12)$ only, resulting in an equation which is independent of $\gamma(12)$. Corrections to scaling in this case were obtained in our previous work [8], and will not be considered further here. For general n , γ cannot be eliminated in favor of $C(12)$, and we will therefore work with γ

instead of $C(12)$. From dimensional considerations we see that $S_0 \sim L^2$ and can be chosen as $S_0 = L^2/\lambda$. This choice effectively defines L , up to an overall constant. For $n \rightarrow \infty$, an expansion in $1/n$ can be performed on $C(\gamma)$, and in this limit $\gamma dC/d\gamma = C + C^3/n + O(1/n^2)$. For $n = \infty$, Mazenko theory reduces to the $n = \infty$ n -vector model for which an exact solution, including the corrections to scaling, is known [8]. Expressing Eq. (6) in terms of γ explicitly leads to

$$\frac{1}{2} \frac{\partial \gamma}{\partial t} = \frac{C_{\gamma\gamma}}{C_\gamma} \left(\frac{\partial \gamma}{\partial r} \right)^2 + \frac{\partial^2 \gamma}{\partial r^2} + \frac{d-1}{r} \frac{\partial \gamma}{\partial r} + \frac{\lambda}{2L^2} \gamma, \quad (7)$$

where $C_\gamma = dC/d\gamma$ etc. Since $C(r, t)$ is a function of $\gamma(r, t)$, the scaling and corrections to scaling can be imposed on $\gamma(r, t)$. In the scaling limit we expect $\gamma(r, t)$ to approach the scaling function $\gamma_0(r/L)$ which is L -independent if all lengths are scaled by L . In this limit therefore one expects $LdL/dt = \text{const}$. Including corrections to scaling in $\gamma(r, t)$ and $L(t)$ as usual [8] we can write

$$\gamma(r, t) = \gamma_0 \left(\frac{r}{L} \right) + L^{-\omega} \gamma_1 \left(\frac{r}{L} \right) + \dots, \quad (8)$$

$$C(r, t) = f_0 \left(\frac{r}{L} \right) + L^{-\omega} f_1 \left(\frac{r}{L} \right) + \dots, \quad (9)$$

$$\frac{dL}{dt} = \frac{1}{2L} + \frac{b}{L^{1+\omega}} + \dots, \quad (10)$$

where

$$f_0 \left(\frac{r}{L} \right) = C(\gamma_0), \quad (11)$$

$$f_1 \left(\frac{r}{L} \right) = \gamma_1 \left(\frac{r}{L} \right) \left[\frac{dC}{d\gamma} \right]_{\gamma=\gamma_0}, \quad (12)$$

and b is a constant. Equating leading and next-to-leading powers of L in the usual way gives

$$\gamma_0'' + \frac{C_{\gamma_0\gamma_0}}{C_{\gamma_0}} \gamma_0'^2 + \left[\frac{x}{4} + \frac{d-1}{x} \right] \gamma_0' + \frac{\lambda}{2} \gamma_0 = 0, \quad (13)$$

$$\begin{aligned} \gamma_1'' + \left[\frac{x}{4} + \frac{d-1}{x} \right] \gamma_1' + \left[\frac{\lambda}{2} + \frac{\omega}{4} \right] \gamma_1 + \frac{b}{2} x \gamma_0' + 2 \frac{C_{\gamma_0\gamma_0}}{C_{\gamma_0}} \gamma_0' \gamma_1' \\ + \left[\frac{C_{\gamma_0\gamma_0\gamma_0}}{C_{\gamma_0}} - \frac{(C_{\gamma_0\gamma_0})^2}{C_{\gamma_0}^2} \right] \gamma_1 \gamma_0'^2 = 0, \end{aligned} \quad (14)$$

with $C_{\gamma_0} = [dC/d\gamma]_{\gamma=\gamma_0}$, etc. The primes indicate derivatives with respect to the scaling variable $x = r/L$.

Equations (13) and (14) are to be integrated numerically subject to appropriate ‘‘initial’’ conditions imposed at $x = 0$. Since $x = 0$ corresponds to $\gamma_0 = 1$, the initial conditions are obtained by considering the regime $\gamma_0 \rightarrow 1$. Using the properties of the hypergeometric functions [20] one can derive relations between $C(\gamma_0)$ and its derivatives as $\gamma_0 \rightarrow 1$. Up to prefactors of order unity, we find in this limit

TABLE I. Exponent λ within Mazenko theory for model A.

n	2	3	4	5
$d=1$	0.301	0.378	0.414	0.433
$d=2$	0.829	0.883	0.912	0.930
$d=3$	1.382	1.413	1.432	1.445

$$C_{\gamma_0\gamma_0}/C_{\gamma_0} \sim [(1-\gamma_0)|\ln(1-\gamma_0)|]^{-1}, \quad n=2, \quad (15)$$

$$C_{\gamma_0\gamma_0\gamma_0}/C_{\gamma_0} \sim [(1-\gamma_0)^2|\ln(1-\gamma_0)|]^{-1}, \quad n=2,$$

$$C_{\gamma_0\gamma_0}/C_{\gamma_0} \sim [1-\gamma_0]^{(n-4)/2}, \quad 2 < n < 4,$$

$$C_{\gamma_0\gamma_0\gamma_0}/C_{\gamma_0} \sim [1-\gamma_0]^{(n-6)/2}, \quad 2 < n < 4,$$

$$C_{\gamma_0\gamma_0}/C_{\gamma_0} \sim |\ln(1-\gamma_0)|, \quad n=4,$$

$$C_{\gamma_0\gamma_0\gamma_0}/C_{\gamma_0} \sim [1-\gamma_0]^{-1}, \quad n=4,$$

$$C_{\gamma_0\gamma_0}/C_{\gamma_0} \rightarrow \text{const}, \quad 4 < n < 6,$$

$$C_{\gamma_0\gamma_0\gamma_0}/C_{\gamma_0} \sim [1-\gamma_0]^{(n-6)/2}, \quad 4 < n < 6,$$

and so on. We have given explicit expressions for $C_{\gamma_0\gamma_0}/C_{\gamma_0}$ and $C_{\gamma_0\gamma_0\gamma_0}/C_{\gamma_0}$ as $\gamma_0 \rightarrow 1$ for the values of n which we are going to study. Using the above results one can show [3] that the small- x behavior of $\gamma_0(x)$ is given by

$$\gamma_0(x) = 1 - \frac{\lambda}{4d} x^2 + \dots \quad (16)$$

for $n \geq 2$, where the limiting forms in Eq. (15) were used to demonstrate that the term involving $C_{\gamma_0\gamma_0}/C_{\gamma_0}$ in Eq. (13) is subdominant as $x \rightarrow 0$ for $n \geq 2$.

For large- x , $\gamma_0 \rightarrow 0$ [also $C(12) \rightarrow 0$] and Eq. (13) becomes linear because in this limit the second term in Eq. (13) is negligible. It is easy to show that two linearly independent solutions of the linearized equation have the asymptotic forms $\gamma_{01} \sim x^{-2\lambda}$ and $\gamma_{02} \sim x^{2\lambda-d} \exp(-x^2/8)$, for $x \rightarrow \infty$. As Eq. (13) is integrated forward from $x = 0$, the large- x solution obtained will in general be a linear combination of γ_{01} and γ_{02} . The amplitudes of γ_{01} and γ_{02} , however, depend on λ . For systems with initial conditions containing only short-range spatial correlations (as is the case for systems quenched from high temperature), a power-law decay is unphysical, and λ is determined by the condition that the coefficient of the power-law term, γ_{01} , must vanish [3]. Note that λ is related to the exponent $\bar{\lambda}$ describing the decay of the autocorrelation function [21] via $\bar{\lambda} = d - \lambda$. Values for λ are given in Table I for $2 \leq n \leq 5$ and $1 \leq d \leq 3$. Comparison of the predicted values of λ with simulations [22] and experiments [23] show reasonable agreement. It can be shown that for $d \rightarrow \infty$ the OJK result ($\lambda = d/2$) is recovered for both scalar [24] and vector [3] cases. The same limit for λ is also obtained for $n \rightarrow \infty$ at arbitrary d .

The correction-to-scaling exponent, ω , is found from Eq. (14) in a similar way to the determination of λ from Eq. (13).

TABLE II. Correction-to-scaling exponent ω within Mazenko theory for model A.

n	2	3	4	5
$d=1$	3.976	3.982	3.990	3.993
$d=2$	3.928	3.946	3.961	3.970
$d=3$	3.930	3.945	3.958	3.966

In order to specify initial conditions for the numerical integration of Eq. (14), we need the small- x behavior of $\gamma_1(x)$. A small- x analysis of Eq. (14) gives $\gamma_1 = b\lambda x^4/16d(d+2) + \dots$, where the results in Eq. (15) were used to show that the last two terms in Eq. (14) are subdominant as $x \rightarrow 0$. The required initial conditions are therefore $\gamma_1(0) = \gamma_1'(0) = 0$. As $x \rightarrow \infty$, the last two terms in Eq. (14) can be neglected. The two linearly independent solutions of the simplified equations have a power-law tail ($\sim x^{-(\omega+2\lambda)}$) and a Gaussian tail [$\sim x^q \exp(-x^2/8)$] for large x , where $q = 2\lambda - d + \omega$ if $\omega > 2$ and $q = 2\lambda - d + 2$ otherwise. Having already found λ , ω is chosen on physical grounds in the same way as λ , namely that the coefficient of the power-law term in the large- x solution should vanish. The values of ω obtained are given in Table II for $2 \leq n \leq 5$ and $1 \leq d \leq 3$. Note that $\omega \rightarrow 4$ for $d \rightarrow \infty$, as the OJK result (and its generalization to vector fields) is recovered in this limit.

After solving Eqs. (13) and (14) for $\gamma_0(x)$ and $\gamma_1(x)$ we use these results to get the scaling function $f_0(x)$ and the correction-to-scaling function $f_1(x)$ from Eqs. (11) and (12). Figure 1 shows the scaling functions $f_0(x)$ and the correction-to-scaling functions $f_1(x)$ for $n=2$ and 3 in 3D. The amplitude of $f_1(x)$ is arbitrary. It is determined by the coefficient b introduced in Eq. (10): the value $b=2$ was used in Fig. 1. The scaling functions and the correction-to-scaling functions do not show strong dependence on n and d for $n \geq 2$. For $n=1$ and $n \geq 2$ the scaling functions are very different, especially in the small- x region. The reason for this is the presence of the sharp interfaces in $n=1$ systems, which lead to a finite slope at the origin in $f_0(x)$ [1] and a cubic small- x behavior in $f_1(x)$ [8]. For $n \geq 2$, the small- x is quadratic for f_0 , and quartic for f_1 , with logarithmic corrections for even n .

Within Mazenko theory the correction-to-scaling exponent ω is nontrivial and depends on both n and d , with $\omega \leq 4$ for all n and d in nonconserved $O(n)$ models. The upper bound of 4 is obtained when $d \rightarrow \infty$ (for any value of n) or $n \rightarrow \infty$ (for any value of d).

A noteworthy feature of Fig. 1 is that the correction-to-scaling function $f_1(x)$ is much larger than $f_0(x)$ at large x (the same feature was found for many of the models studied in [8]). This means that, in fitting data, scaling violations at large- x should be given less weight in choosing fitting parameters [e.g., the scale length $L(t)$] than violations at small or intermediate x , because corrections to scaling are larger there.

IV. THE ONE-DIMENSIONAL XY MODEL

An exact solution of this model was first presented by Newman *et al.* [22]. The solution yields an ‘‘anomalous’’

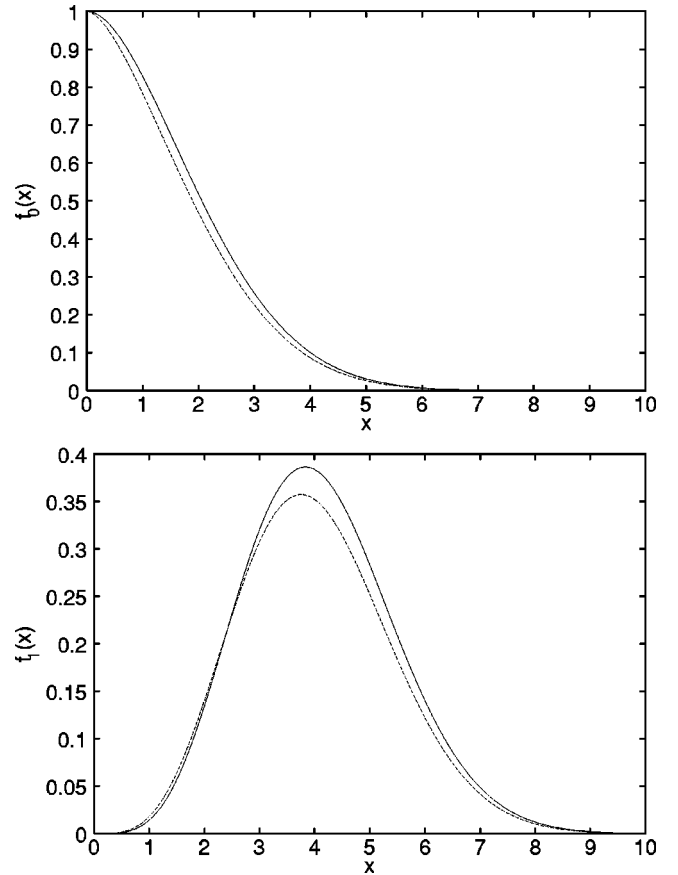


FIG. 1. The scaling function $f_0(x)$ and the correction-to-scaling function $f_1(x)$ for nonconserved order parameter. Continuous and broken lines correspond to $d=n=3$ and $d=3, n=2$, respectively.

growth law, $L \sim t^{1/4}$, for the characteristic length exhibited by the pair correlation function, compared with the usual $L \sim t^{1/2}$ growth law of nonconserved models. Mazenko theory does not predict this growth law, for the simple reason that the theory has been built in such way that it might be expected to give qualitatively correct results only for systems with topological defects (i.e., $n \leq d$), since the n -component auxiliary field $\vec{m}(\mathbf{r}, t)$ is defined in terms of the underlying defect structure. Despite this, the theory does a reasonable job of accounting for the behavior of systems with $n > d$, and in fact becomes exact in the limit $n \rightarrow \infty$. However, systems with $n = d + 1$, which can support topological textures, are poorly treated by this approach.

An exact solution for the nonconserved $n=2, d=1$ system is possible because the equation of motion for the order parameter becomes linear in the angle representation, $\vec{\phi} = (\cos \theta, \sin \theta)$, which is natural in the hard-spin limit, where $\vec{\phi}^2 = 1$. In this limit the free energy functional is simply $F = (1/2) \int dx (d\vec{\phi}/dx)^2 = (1/2) \int dx (d\theta/dx)^2$. The zero-temperature equation of motion for model A, $\partial \vec{\phi} / \partial t = -\delta F / \delta \vec{\phi}$, becomes, in the angle representation,

$$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial x^2}, \quad (17)$$

which is a diffusion equation for the phase angle θ . Thus one

characteristic length scale is the ‘‘phase diffusion length,’’ $L_\theta = t^{1/2}$, but this is not the scale which characterizes the pair correlation function.

Equation (17) can be solved in Fourier space to give $\theta_k(t) = \theta_k(0)\exp(-k^2t)$. In evaluating quantities of interest such as correlation functions, one needs to specify the initial conditions. The probability distribution, $P([\theta_k(0)])$, for $\theta_k(0)$ is conveniently chosen to be Gaussian $P([\theta_k(0)]) \propto \exp[-\frac{1}{2}\sum_k \beta_k \theta_k(0)\theta_{-k}(0)]$. The choice $\beta_k = \xi_0 k^2/2$ is made as it gives the initial condition $C(r,0) = \exp(-r/\xi_0)$ for the order-parameter correlation function, which is the appropriate form for systems quenched from an equilibrium disordered state with correlation length ξ_0 . The equal-time correlation function is given by

$$C(r,t) = \langle \vec{\phi}(x,t) \cdot \vec{\phi}(x+r,t) \rangle = \langle \cos[\theta(x+r,t) - \theta(x,t)] \rangle. \quad (18)$$

Using the Gaussian probability distribution for $\theta_k(0)$ Eq. (18), with the dynamics (17) gives

$$C(r,t) = \exp\left(-\sum_k \frac{1}{\beta_k} \exp(-2k^2t)[1 - \cos kr]\right). \quad (19)$$

Since the characteristic value of k in the integral is of order $t^{-1/2}$, and we anticipate (see below) the growth law $L(t) \sim t^{1/4}$, which sets the characteristic scale of r in $C(r,t)$, it follows that the scaling limit and the corrections to it can be obtained from a power-series expansion of $\cos(kr)$ in Eq. (19), since the characteristic value of kr is small (of order $t^{-1/4}$) at late times. Retaining the leading and next-to-leading terms in the exponent, and evaluating the sums over k , gives

$$\begin{aligned} C(r,t) = \exp\left[-\frac{r^2}{2\xi_0(2\pi t)^{1/2}} + \frac{r^4}{96\xi_0(2\pi)^{1/2}t^{3/2}}\right. \\ \left.+ O\left(\frac{r^6}{\xi_0 t^{5/2}}\right)\right] = \exp\left[-\frac{y^2}{2(2\pi)^{1/2}}\right] \\ \times \left[1 + \frac{\xi_0^2}{L^2} \frac{y^4}{96(2\pi)^{1/2}} + O\left(\frac{\xi_0^4}{L^4}\right)\right], \quad (20) \end{aligned}$$

where $y = r/L$ is the scaling variable and the coarsening scale $L(t) = \xi_0^{1/2} t^{1/4}$. The correction-to-scaling exponent is $\omega = 2$.

This growth law is rather unusual since the generic form of the growth law for nonconserved fields is $L(t) \sim t^{1/2}$. In this model ω is found to be trivial while within Mazenko theory ω is nontrivial. There are two fundamental length scales in this problem, namely the phase coherence $t^{1/2}$ and the correlation length ξ_0 associated with the initial conditions. The coarsening scale $L(t)$ of the pair correlation function is the geometric mean of these two lengths. Note that the pair correlation function has a strong dependence on ξ_0 , which is not ‘‘forgotten’’ at late times. This sensitivity to initial conditions is absent in other models, such as $n = \infty$ vector model, where the initial conditions drop out at late times. In the conserved 1D XY model also, simulation results gives $L \approx t^{1/6}$ [14] instead of the $L \sim t^{1/4}$ behavior expected in higher dimensions [10], suggesting that this ‘‘anomalous’’

behavior may be present there also. Although no exact solution is known for the conserved case, heuristic arguments, based on the role of the two characteristic lengths, can account for the observed $t^{1/6}$ growth [25].

V. CONSERVED $O(n)$ MODEL

The dynamical scaling properties of systems with a conserved order parameter (model B) with $O(n)$ symmetry is studied using Mazenko theory. Naive application of this theory does not give correct growth law $L \sim t^{1/3}$ for scalar fields (the bulk diffusion field must be included in order to get the correct law [26]). Here, however, we will only consider systems with $n \geq 2$. For model B systems, Eq. (4) becomes

$$\frac{1}{2} \frac{\partial C(12)}{\partial t} = -\nabla^2 \left[\nabla^2 C(12) + \alpha(t) \gamma \frac{dC(12)}{d\gamma} \right], \quad (21)$$

with $\alpha(t) = 1/2S_0$. For Eq. (21) to have a scaling solution it is clear that $\alpha \sim 1/L^2$ and $L \sim t^{1/4}$. The latter is the correct growth law for $n \geq 2$, but for $n = 2$, $d > 2$ there are logarithmic corrections [10] which Eq. (21) fails to predict. We will first consider the case where n is very large. In this case an expansion in $1/n$ can be made in Eq. (21). For large n , $C(\gamma) \sim \gamma - \gamma(1 - \gamma^2)/2n + O(1/n^2)$ and $\gamma[dC(12)/d\gamma] = C + C^3/n + O(1/n^2)$. With the above truncations, Eq. (21) can be written as

$$\frac{1}{2} \frac{\partial C(12)}{\partial t} = -\nabla^2 \left[\nabla^2 C(12) + \alpha(t) \left(C + \frac{C^3}{n} \right) \right], \quad (22)$$

correct to order $1/n$.

It is worth mentioning that the C^3/n term is essential for scaling to be recovered at finite n . For n strictly infinite the C^3/n term is absent and ‘‘multiscaling’’ is obtained [11]. For arbitrary n , an expansion in powers of C can be made. Truncating the expansion at order C^3 leads back to Eq. (22) but with n replaced by an effective n^* , given by $n^* = (n + 2)a_n^2$ with $a_n = n[B((n+1)/2, 1/2)]^2/2\pi$ [4].

Dimensional analysis of Eq. (22) requires $\alpha(t) = \alpha/L^2$, which defines L . Including the leading corrections to scaling as usual we write

$$C(r,t) = f_0(r/L) + L^{-\omega} f_1(r/L) + \dots, \quad (23)$$

$$dL/dt = 1/4L^3 + b/L^{\omega+3} + \dots, \quad (24)$$

where b fixes the amplitude of $f_1(r/L)$. Inserting these expansions into Eq. (22) and comparing terms of leading order, $O(1/L^4)$, and next-to-leading order, $O(1/L^{4+\omega})$, gives

$$\frac{x}{8} \frac{df_0}{dx} = \nabla_x^2 \left[\nabla_x^2 f_0 + \alpha \left(f_0 + \frac{f_0^3}{n} \right) \right], \quad (25)$$

$$\frac{x}{8} \frac{df_1}{dx} + \frac{\omega}{8} f_1 + \frac{bx}{2} \frac{df_0}{dx} = \nabla_x^2 \left[\nabla_x^2 f_1 + \alpha \left(f_1 + \frac{3f_0^2 f_1}{n} \right) \right], \quad (26)$$

where $\nabla_x^2 = d^2/dx^2 + [(d-1)/x]d/dx$.

For general n one must solve Eq. (21) with $C(r,t)$ given by Eq. (5). However, the singularities of $C(\gamma)$ and its de-

TABLE III. Values for the eigenvalues α , β , μ , and ω within Mazenko theory for model B.

n	α	β	μ	ω
2	1.54880435	-0.3336250	0.227495	2.4613967
5	1.72743447	-0.3179775	0.225025	2.0667992
20	2.01748270	-0.3292250	0.214515	1.1290901
50	2.179330049	-0.3487125	0.206515	0.5029987

rivatives at $\gamma=1$ introduce some numerical difficulties. Instead, therefore, we solve Eq. (22) which is valid for large n . For general n , an expansion in C up to C^3 , leading to Eq. (22) with an effective n^* [4], gives scaling functions which are in fairly good agreement with simulation results [4,15].

In solving Eq. (25) numerically, one must know the boundary conditions. These are provided by small- x and large- x analyses. For small- x , the series expansion $f_0 = 1 + \sum_{r=1}^{\infty} \beta_r x^r$, substituted into Eq. (25), gives $f_0 = 1 + \beta x^2 - (1 + 3/n)\alpha \beta x^4/4(2+d) + \dots$, with $\beta_2 = \beta$. Numerical integration can therefore be performed on Eq. (25) with initial conditions $f_0(0) = 1$, $f_0''(0) = 2\beta$, $f_0'(0) = f_0'''(0) = 0$. Both α and β are undetermined parameters.

For the large- x analysis, we impose the physical condition that $f_0(x) \rightarrow 0$ for $x \rightarrow \infty$. This leads to the linearized version of Eq. (25) given by

$$\frac{x}{8} \frac{df_0}{dx} = \nabla_x^2 [\nabla_x^2 f_0 + \alpha f_0]. \quad (27)$$

There are four linearly independent solutions of Eq. (27), with the general asymptotic form

$$f_0(x) \sim F_0 x^c \exp(-Bx^v - Ax^s). \quad (28)$$

The first solution is the constant solution, corresponding to $A = c = B = 0$. It satisfies Eq. (27) by inspection. The other three solutions are obtained by substituting Eq. (28) into Eq. (27) and carrying out an asymptotic large- x analysis, leading to the relations

$$v = 4/3,$$

$$s = 2/3,$$

$$B^3 = -1/8v^3,$$

$$A = 64\alpha B^2/9,$$

$$c = -2d/3.$$

The three different solutions correspond to the three solutions for B , one real, two complex. The real solution, $B = -1/2v = -3/8$, leads to an exponentially diverging solution for f_0 :

$$f_0(x) \sim F_0 x^{-2d/3} \exp(3x^{4/3}/8 - \alpha x^{2/3}), \quad (29)$$

while the two complex roots, $B = 3(1 \pm i\sqrt{3})/16$, generate two solutions which can be combined to give an exponentially decaying solution with oscillatory behavior

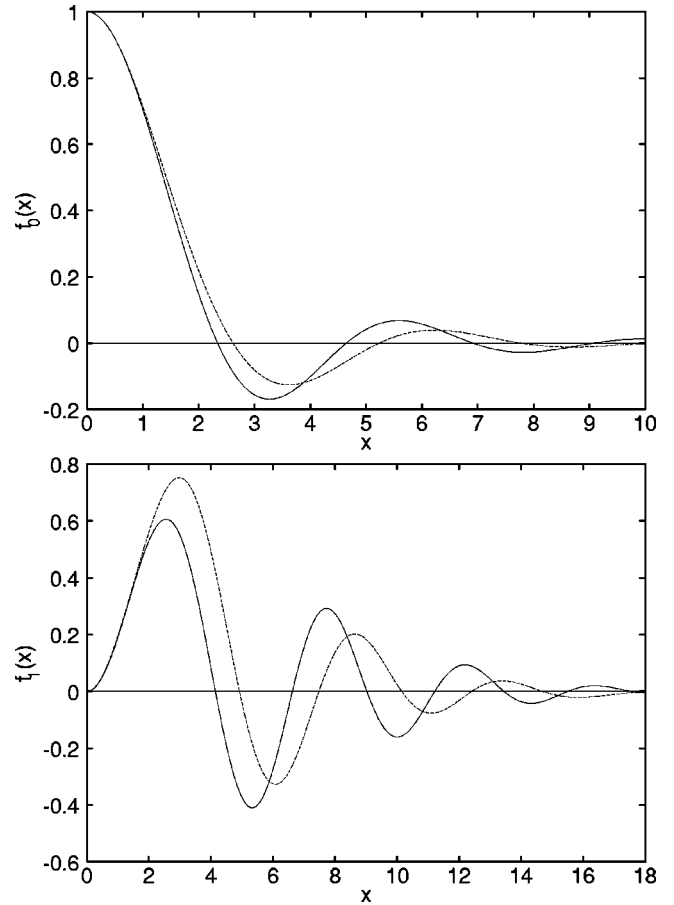


FIG. 2. Same as in Fig. 1, but for conserved order parameter. Continuous and broken lines correspond to $d=3$, $n=20$, and $d=3$, $n=2$, respectively (note the different scales for the x axes in the upper and lower plots).

$$f_0(x) \sim F_0 x^{-2d/3} \exp\left(-\frac{3x^{4/3}}{16} + \frac{\alpha x^{2/3}}{2}\right) \times \cos\left(\frac{3\sqrt{3}x^{4/3}}{16} + \frac{\alpha\sqrt{3}x^{2/3}}{2} + \varphi_0\right), \quad (30)$$

where F_0 and φ_0 are arbitrary constants.

Just as in the model A case, where λ was fixed by imposing physical conditions on the large- x solution, also in this case we have an eigenvalue problem in which two parameters α and β are chosen to eliminate the unphysical constant solution and the exponentially diverging solution. The same problem is encountered in model B with a scalar order parameter [6]. Applying the procedure described in [4,6] it is possible to determine α and β .

Turning now to the corrections to scaling, we consider first the four linearly independent large- x solutions for the linearized form of Eq. (26). These are a power law solution, $f_1(x) \sim x^{-\omega}$, an exponentially growing solution, $\sim x^p \exp(3x^{4/3}/8 - \alpha x^{2/3})$, and two decaying solutions that can be combined in the form

$$f_1(x) \sim x^p \exp\left(\frac{-3x^{4/3}}{16} + \frac{\alpha x^{2/3}}{2}\right) \times \cos\left(\frac{3\sqrt{3}x^{4/3}}{16} + \frac{\alpha\sqrt{3}x^{2/3}}{2} + \varphi_1\right), \quad (31)$$

where φ_1 is arbitrary, and $p=(\omega-2d)/3$ if $\omega>4$ and $p=(4-2d)/3$ otherwise. The small- x solution is $f_1(x)=\mu x^2 - \alpha\mu(1+3/n)x^4/4(d+2)+\dots$. Therefore Eq. (26) is solved numerically with initial conditions $f_1''(0)=2\mu$, $f_1(0)=f_1'(0)=f_1'''(0)=0$. The two parameters μ and ω are as yet undetermined. They are fixed in the same way as α and β , by requiring that an oscillatory, exponentially decaying solution is recovered as $x\rightarrow\infty$.

Values for α , β , μ , and ω in 3D for $n=2, 5, 10, 20$, and 50 are shown in Table III (For $n=2$, the effective $n^*=\pi^2/4$ has been used). The functions $f_0(x)$ and $f_1(x)$ are displayed in Fig. 2 for $n=2$ and 20 in 3D. Again b has been set to $b=2$ without loss of generality.

The most important result to be extracted from Table III is that the value of ω decreases as n increases. This behavior is quite different from model A, where ω increases asymptotically to 4 as n increases. It seems from Table III that ω probably tends to zero for $n\rightarrow\infty$, although an analytical determination of the correction to scaling for n large but finite, analogous to the treatment of the leading scaling function in [12], has not yet been realized.

Comparison of the scaling and correction-to-scaling functions displayed in Fig. 2 reinforces a point made in connection with the nonconserved systems, namely that the correction to scaling become large (relative to the scaling function itself) at large values of the scaling variable x . As noted before, this suggests that in carrying out scaling analyses of data, more attention should be paid to small and intermediate values of x , where corrections to scaling can be expected to be (relatively) smaller, than to large x . Indeed, for the nonconserved case (Fig. 1) the correction to scaling has its maximum at a point where the scaling function is already quite small (around 0.1).

VI. SUMMARY

Corrections to scaling associated with a nonscaling initial condition have been studied in $O(n)$ models within the Gaussian closure scheme of Mazenko. We have calculated both the correction-to-scaling function, $f_1(x)$, and the asso-

ciated correction-to-scaling exponent, ω , for both nonconserved and conserved fields. In both cases Mazenko theory suggests that ω is nontrivial, depending on the nature of the dynamics involved, the dimensionality, d , of the system and the number of order parameter components, n . For nonconserved fields the value of ω tends to the limiting value 4 for $n\rightarrow\infty$ with d fixed, and for $d\rightarrow\infty$ with n fixed. In the latter limit, the Mazenko theory reduces [3,24] to the OJK theory [7] and its generalizations [19], believed to become exact as $d\rightarrow\infty$ [27].

The 1D XY model is anomalous in that it exhibits a different growth law from the standard one for nonconserved dynamics, and the correction-to-scaling exponent is simple ($\omega=2$). In this model quantities of interest, such as the correlation function $C(r,t)$, retain ‘‘memory’’ of the initial conditions even in the scaling limit.

In studying the conserved $O(n)$ model, an expansion in $1/n$ was used which is valid for large n . This approach was used to find the correction-to-scaling function $f_1(x)$ and the exponent ω for $n=5, 20$, and 50 in 3D. For $n=2$, an expansion in C up to C^3 was made. In the latter case, a comparison [4] between leading-order scaling results and simulations shows very good agreement despite the wrong growth law (i.e., without the logarithmic corrections predicted for $n=2$ [10]). In conserved systems ω decreases as n increases, raising the question of whether $\omega\rightarrow 0$ or approaches some limiting value as n becomes very large. We have as yet been unable to find $f_1(x)$ and ω analytically in the limit of large but finite n —this remains an interesting open question.

The main lesson for the analysis of experimental and simulation data is that corrections to scaling can be expected to be relatively small at small and intermediate scaling variable $x(=r/L)$, suggesting that this region be given more weight than large x in fitting (or collapsing) data.

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