

Corrections to scaling in phase-ordering kinetics

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(Received 19 September 1997)

The leading correction to scaling associated with departures of the initial condition from the scaling morphology is determined for some soluble models of phase-ordering kinetics at zero temperature. The result for the pair correlation function has the form $C(r,t) = f_0(r/L) + L^{-\omega} f_1(r/L) + \dots$, where L is a characteristic length scale extracted from the energy. The correction-to-scaling exponent ω has the value $\omega=4$ for the $d=1$ Glauber model, the n -vector model with $n=\infty$, and the approximate theory of Ohta, Jasnow, and Kawasaki. For the approximate Mazenko theory, however, ω has a non-trivial value: $\omega=3.8836, \dots$ for $d=2$, and $\omega=3.9030, \dots$ for $d=3$. The correction-to-scaling functions $f_1(x)$ are also calculated. [S1063-651X(98)09402-3]

PACS number(s): 64.60.Cn

I. INTRODUCTION

The phenomenon of phase-ordering kinetics has attracted considerable attention in recent years [1]. It is now well established that, except in certain exceptional circumstances, a scaling regime develops at late times, in which the order-parameter morphology is time independent up to one overall time-dependent length scale $L(t)$. This means, for example, that the equal-time pair correlation function of the order parameter, $C(r,t) = \langle \phi(\mathbf{x} + \mathbf{r}, t) \phi(\mathbf{x}, t) \rangle$ has the asymptotic scaling form $C(r,t) = f[r/L(t)]$. Relatively little attention, however, has been devoted to the study of how the scaling regime is approached, i.e., the form of ‘‘corrections to scaling’’ in phase-ordering kinetics. In particular, an understanding of corrections to scaling is important in interpreting experimental or simulation data, and in extracting asymptotic scaling exponents and functions.

This article attempts a systematic study of corrections to scaling. We show that there is a correction-to-scaling exponent ω associated with the deviations of the order parameter morphology from the scaling morphology, i.e., with the fact that the initial state is not in general the scaling state. Pre-supposing a suitable definition of $L(t)$, which will require some discussion, the leading corrections to scaling in the pair correlation function enter in the form $C(r,t) = f_0(r/L) + L^{-\omega} f_1(r/L)$, where $f_0(x)$ is the ‘‘scaling function’’ and $f_1(x)$ the ‘‘correction-to-scaling function.’’ There are indications that ω is, in general, a *nontrivial exponent* of phase-ordering kinetics. Although for most of the simple, exactly soluble models presented here it has the value $\omega=4$, we find that it takes nontrivial values within an approximate calculation for more realistic models. The models considered are the one-dimensional (1D) Glauber model, the $O(n)$ nonlinear sigma model for $n=\infty$, the 1D time-dependent Ginzburg-Landau (TDGL) equation, the Ohta-Jasnow-Kawasaki (OJK) approximation [2] for the general TDGL equation, and lastly the Mazenko approximation [3]. It is the last of these that yields nontrivial values for ω . In fact ω enters the theory in a similar way to the exponent $\bar{\lambda}$, which describes the decay of the autocorrelation function and is known to be nontrivial [4]. For the 1D TDGL equation, we find that the approach to

the scaling state is much faster than for the other models: for typical initial conditions the corrections to scaling vanish exponentially fast as a function of the smallest domain size.

It is important to recognize that corrections to scaling can have more than one origin. For a scalar order parameter, for example, in which the morphology is specified by the locations of the domain walls, the scaling regime requires that the domain scale $L(t)$ be much larger than the width ξ of the walls. Therefore one expects a correction to scaling associated simply with the nonzero width of domain walls, and entering as a power of ξ/L . This is a distinct contribution from the one considered here, which is associated with departures from the scaling morphology in the initial condition. This latter contribution will survive even in the thin wall limit described by, for example, the Allen-Cahn theory [1,6] in which infinitely thin interfaces are driven by their local curvature. Throughout this paper we restrict ourselves to this thin-wall limit, or the corresponding ‘‘hard-spin’’ limit (or nonlinear sigma model) for a vector order parameter. This leads to useful simplifications.

Another source of corrections to scaling is thermal fluctuations. All the results presented here are for quenches to zero temperature. For those systems that exhibit a phase transition with a nonzero T_c , the leading scaling behavior for a quench to temperature T is believed to be the same, for all $T < T_c$, as for a quench to $T=0$ (apart from some temperature-dependent amplitudes) due to the ‘‘irrelevance’’ of thermal fluctuations below T_c [1,7]. Thermal fluctuations at $T > 0$, however, provide their own corrections to scaling, which will not be discussed explicitly here. We simply note that, in the temperature-related corrections to scaling, the temperature enters through the combination T/L^y , where $y = d-1$ for scalar fields and $d-2$ for vector fields [1,7]. This implies that if the leading ‘‘thermal’’ correction to scaling is linear in T , for example, the thermal correction-to-scaling exponent will be y . Such a case is realized in the nonconserved dynamics of the $O(n)$ model with $n \geq 2$ [7], as may be shown explicitly in the limit $n \rightarrow \infty$ [8].

The paper is organized as follows. Section II deals with the 1D Glauber model, and introduces some general concepts. The large- n vector model, 1D TDGL equation, OJK theory, and Mazenko theory, are covered in Secs. III–VI,

respectively. Section VII concludes with a discussion and summary.

II. THE ONE-DIMENSIONAL GLAUBER MODEL

In the continuum limit, the equation of motion for the pair correlation function $C(r,t)$ has the form [5]

$$\partial_t C = \partial_r^2 C, \quad C(0,t) = 1. \quad (1)$$

The constraint $C(0,t) = 1$ can be built in through a source term at $r=0$, i.e., we modify the equation of motion to

$$\partial_t C = \partial_r^2 C + A(t) \delta(r), \quad (2)$$

where $A(t)$ is chosen to satisfy the constraint. Let us define L to be the average domain size. Then for $r \ll L$, we have

$$C(r,t) = 1 - 2\rho_w |r| = 1 - 2|r|/L, \quad (3)$$

where $\rho_w = 1/L$ is the density of domain walls, and we have allowed for the possibility of either one or zero walls in an interval of length r . Equation (3) is then correct to order r .

Integrating Eq. (2) across an infinitesimal interval around $r=0$, and comparing with Eq. (3), gives $A = 4/L$. Putting this into Eq. (2), and writing $C(r,t)$ in terms of r and L in the form

$$C(r,t) = f(r/L, L) \quad (4)$$

gives the following equation for $f(x, L)$:

$$\dot{L} \frac{\partial f}{\partial L} = \frac{1}{L^2} f'' + \frac{\dot{L}}{L} x f' + \frac{4}{L^2} \delta(x), \quad (5)$$

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

In the limit $L \rightarrow \infty$, we expect $f(x, L)$ to approach the L -independent scaling function $f_0(x)$. Balancing powers of L on the right of Eq. (5) then implies $\dot{L}L = \text{const}$, i.e., $L \propto t^{1/2}$. Including the leading correction to scaling, of relative order $L^{-\omega}$, we write

$$\dot{L} = a/L + b/L^{1+\omega} + \dots, \quad (6)$$

$$f(x, L) = f_0(x) + L^{-\omega} f_1(x) + \dots \quad (7)$$

in Eq. (5), and equate terms of leading (L^{-2}) and next-to-leading ($L^{-2-\omega}$) order. This gives

$$f_0'' + a x f_0' + 4 \delta(x) = 0, \quad (8)$$

$$f_1'' + a x f_1' + a \omega f_1 + b x f_0' = 0. \quad (9)$$

Integrating Eq. (8) with the boundary conditions $f(0) = 1$, $f'(0+) = -2$ [from Eq. (3)] gives (for $x \geq 0$)

$$a = 2\pi, \quad (10)$$

$$f_0(x) = \text{erfc}\left(\sqrt{\frac{a}{2}} x\right). \quad (11)$$

Equation (9) for f_1 becomes

$$f_1'' + a x f_1' + a \omega f_1 = \bar{b} x \exp(-a x^2/2), \quad (12)$$

where $\bar{b} = b(2a/\pi)^{1/2} = 2b$. Writing $f_1(x) = \exp(-a x^2/2) g(x)$ gives

$$g'' - a x g' + a(\omega - 1)g = \bar{b} x. \quad (13)$$

What are the boundary conditions on $g(x)$? Clearly $g(0) = 0$, because $C(0,t) = 1$ is already implemented by $f_0(0) = 1$. Similarly, the condition $\partial_r C(r,t)|_{r=0} = -2/L$, from Eq. (3), is already guaranteed by $f_0'(0) = -2$, so $g'(0) = 0$. Furthermore, Eq. (13) then gives $g''(0) = 0$, implying that the series expansion for $g(x)$ starts at $O(x^3)$. Inserting the series solution $g(x) = \sum_{n=3}^{\infty} g_n x^n$ gives $g_3 = \bar{b}/6$, and the recurrence relation $g_{n+2} = [a(n+1-\omega)/(n+1)(n+2)]g_n$ for the higher-order odd coefficients, all even coefficients vanishing. In order that $f_1(x)$ decrease faster than a power law for large x , as required on physical grounds for initial conditions with only short-range correlations, the series expansion for $g(x)$ must terminate. This gives the condition $\omega = n+1 = 4, 6, 8, \dots$. We conclude that the leading correction-to-scaling exponent for the 1D Glauber model is

$$\omega = 4, \quad (14)$$

with corresponding correction-to-scaling function

$$f_1(x) = (\bar{b}/6) x^3 \exp(-a x^2/2). \quad (15)$$

The same result can be obtained either from a direct solution of Eq. (1) for a general initial condition [5], or from Glauber's solution [9] of the lattice model.

III. THE LARGE- N LIMIT OF THE $O(N)$ MODEL

It is convenient to work with spins of fixed length, i.e., with the nonlinear sigma model, to avoid additional (uninteresting) corrections to scaling associated with the gradual saturation in the length of the spins as the coarsening proceeds. The nonconserved dynamics of the $O(n)$ nonlinear sigma model is described by the equation [10]

$$\partial_t \vec{\phi} = \nabla^2 \vec{\phi} + (\nabla \vec{\phi})^2 \vec{\phi}, \quad (16)$$

corresponding to the equation $\partial_t \vec{\phi} = -\delta F / \delta \vec{\phi}$, with free energy $F = \frac{1}{2} \int d^d x (\nabla \vec{\phi})^2$, subject to the constraint $[\vec{\phi}(\mathbf{x}, t)]^2 = 1$.

In the limit $n \rightarrow \infty$ we can replace $(\nabla \vec{\phi})^2$ by its mean in the usual way [10]. Let us call this mean $\alpha(t)$. In the scaling regime, dimensional analysis gives $\alpha(t) = \lambda/2L^2$, where λ is a constant. The energy density is just $\epsilon(t) = \alpha(t)/2 = \lambda/4L^2$. It is, in fact, convenient to *define* $L(t)$ through this relation for all times t (in the same spirit as the 1D Glauber model). Then multiplying Eq. (16) by $\phi(\mathbf{x} + \mathbf{r}, t)$ and averaging over initial conditions gives the equation

$$\frac{1}{2} \frac{\partial C}{\partial t} = \nabla^2 C + \frac{\lambda}{2L^2} C \quad (17)$$

for the pair correlation function $C(r, t)$.

In analogy to our treatment of the 1D Glauber model we write $C(r,t)=f(r/L,L)$. Then Eq. (17) becomes the following equation for $f(x,L)$:

$$\frac{\dot{L}}{2} \frac{\partial f}{\partial L} = \frac{1}{L^2} \left(f'' + \frac{d-1}{x} f' + \frac{\lambda}{2} f \right) + \frac{\dot{L}}{2L} x f'. \quad (18)$$

Inserting the forms (6) and (7) (taking $a=1/2$ without loss of generality), and equating coefficients of the terms in L^{-2} and $L^{-(2+\omega)}$ as before gives

$$f_0'' + \left(\frac{d-1}{x} + \frac{x}{4} \right) f_0' + \frac{\lambda}{2} f_0 = 0, \quad (19)$$

$$f_1'' + \left(\frac{d-1}{x} + \frac{x}{4} \right) f_1' + \left(\frac{\lambda}{2} + \frac{\omega}{4} \right) f_1 + \frac{b}{2} x f_1' = 0. \quad (20)$$

Consider first f_0 . The two linearly independent solutions have large- x behavior $\sim x^{-2\lambda}$ and $\sim \exp(-x^2/8)$. The power-law term must be absent for a physical solution corresponding to an initial condition with only short-range correlations. Setting $f_0(x) = \exp(-x^2/8) g_0(x)$ in Eq. (19) gives $g_0'' + [(d-1)/x - x/4] g_0' + (\lambda/2 - d/4) g_0 = 0$. The boundary conditions are $g_0(0)=1$, $g_0'(0)=0$ (the latter being required by the differential equation, to avoid a singularity at $x=0$). To retain the Gaussian tail in f_0 , the series solution for g_0 must terminate. This fixes $\lambda = d/2 + n$ ($n=0,1,2,\dots$), with a corresponding set of polynomial solutions for g_0 , the first two of which are $g_0^{(0)}=1$, and $g_0^{(1)}=1-x^2/4d$. An explicit solution of C for a general initial condition shows that these different scaling solutions are selected by the small- k behavior of the structure factor, $S(\mathbf{k},t)$ [the Fourier transform of $C(\mathbf{r},t)$], at $t=0$. The polynomial solution $g_0^{(n)}$ corresponds to an initial condition with $S(\mathbf{k},0) \propto (k^2)^n$ for $k \rightarrow 0$. A generic initial condition, therefore, selects the $n=0$ solution, i.e., $\lambda = d/2$ and $f_0(x) = \exp(-x^2/8)$.

Consider now the correction-to-scaling function f_1 . Putting $f_1(x) = \exp(-x^2/8) g_1(x)$ in Eq. (20), with $\lambda = d/2$ and $f_0(x) = \exp(-x^2/8)$, gives

$$g_1'' + \left(\frac{d-1}{x} - \frac{x}{4} \right) g_1' + \frac{\omega}{4} g_1 = \frac{b}{8} x^2. \quad (21)$$

Again one seeks a series solution for $g_1(x)$. The boundary conditions $g_1(0)=0=g_1'(0)$ imply that the series has the form $g_1(x) = \sum_{n=2}^{\infty} g_n x^n$. Substituting this into the differential equation one readily finds that $g_n=0$ for n odd, $g_2=0$, $g_4 = b/[32(d+2)]$, and $g_{n+2} = [(n-\omega)/4(n+2)(n+d)] g_n$ for even $n \geq 4$. For a physically sensible large- x behavior, the series must terminate, just as in the one-dimensional Glauber model. This requires $\omega=4,6,8,\dots$. For each such ω , there is a corresponding correction-to-scaling function. The generic case, corresponding to short-range correlations in the initial condition, is the smallest value of ω , i.e., $\omega=4$, with $g_1(x) = bx^4/32(d+2)$. The correction-to-scaling function is then

$$f_1(x) = \frac{bx^4}{32(d+2)} \exp\left(-\frac{x^2}{8}\right). \quad (22)$$

The value of ω for the $n=\infty$ limit, $\omega=4$, is thus identical to that of the 1D Glauber model, raising the question of whether this could be a general result for models with non-conserved dynamics. Indeed, the Ohta-Jasnow-Kawasaki theory discussed in Sec. V gives the same result. The related approach of Mazenko (Sec. VI), however, gives a different, and indeed nontrivial, result. In the following section, we discuss another model with $\omega \neq 4$.

IV. THE ONE-DIMENSIONAL TDGL EQUATION

Another exactly soluble model (in a suitable limit) is the time-dependent Ginzburg-Landau (or TDGL) equation in one dimension. This reads

$$\partial_t \phi = \partial_x^2 \phi - V'(\phi), \quad (23)$$

where $\phi(x,t)$ is the order-parameter field and $V(\phi)$ is a potential function, with a symmetric double-well structure. For convenience, we can take the minima of V to be at $\phi = \pm 1$. Equation (23) represents the simple relaxational dynamics $\partial_t \phi = -\delta F/\delta \phi$, with free-energy functional $F[\phi] = \int dx [(\partial_x \phi)^2/2 + V(\phi)]$. In higher dimensions, this equation can be reduced to the standard model of curvature-driven growth [6,1], whereby the domain walls move with a velocity proportional to their local curvature. In one dimension, of course, the domain walls are points, and domain coarsening is driven by the exponentially weak forces between adjacent walls, mediated by the exponential tails of the domain-wall profiles.

For the case of interest, where the typical domain size L is large compared to the width ξ of a wall, the closest pair of domain walls annihilate while the remaining walls hardly move at all, leading to the following simplified model [11]. The smallest domain is combined with its two neighbors to form a new single domain. This process is then repeated. Eventually the system reaches a scaling state in which the distribution $P(l,a)$ of domain sizes l , when the smallest domain size is a , has the scaling form $P(l,a) = a^{-1} f(l/a)$.

An important feature of this process is that if the domain sizes are initially uncorrelated they remain uncorrelated, because the merging of three domains into a single domain introduces no correlations [12,13]. It is then straightforward to derive an equation of motion for the evolution of the distribution $P(l,a)$ as a increases [11–13]:

$$\begin{aligned} \partial P/\partial a = & -P(a,a) \delta(l-a) + \theta(l-3a) P(a,a) \\ & \times \int_a^{l-2a} P(l',a) P(l-l'-a,a) dl'. \end{aligned} \quad (24)$$

Introducing the Laplace transform with respect to l , $\phi(p,a) = \int_0^\infty P(l,a) \exp(-pl) dl$, gives

$$\partial \phi/\partial a = -P(a,a) \exp(-pa) (1 - \phi^2). \quad (25)$$

This equation can, in fact, be integrated exactly [14] but, in the spirit of the previous sections, we shall first look for solutions of the form

$$\phi(p,a) = \phi_0(pa) + \frac{1}{a^\omega} \phi_1(pa) + \dots, \quad (26)$$

$$P(a,a) = \frac{1}{a}f_0(1) + \frac{1}{a^{1+\omega}}f_1(1) + \dots, \quad (27)$$

where $f_0(x)$, $f_1(x)$ are the scaling and correction-to-scaling functions for the domain-size distribution, ϕ_0 , ϕ_1 are the corresponding Laplace transforms, and ω is the correction-to-scaling exponent as usual. Inserting Eqs. (26) and (27) into Eq. (25), and equating leading and subleading terms gives

$$\frac{d\phi_0}{ds} = -f_0(1) \frac{\exp(-s)}{s} (1 - \phi_0^2), \quad (28)$$

$$\begin{aligned} \frac{d\phi_1}{ds} = & \left(\frac{\omega}{s} + 2f_0(1) \frac{\exp(-s)}{s} \phi_0 \right) \phi_1 \\ & - f_1(1) \frac{\exp(-s)}{s} (1 - \phi_0^2), \end{aligned} \quad (29)$$

where $s=pa$. With the boundary conditions $\phi_0(\infty)=0$ (which follows from the definition of ϕ_0) and $\phi_1(0)=0$ [which follows from the normalization of $P(l,a)$], these equations can be integrated to give

$$\phi_0(s) = \tanh \left(f_0(1) \int_s^\infty \frac{dt}{t} \exp(-t) \right), \quad (30)$$

$$\phi_1(s) = f_1(1) s^\omega [1 - \phi_0^2(s)] \int_s^\infty \frac{dt}{t^{1+\omega}} \exp(-t). \quad (31)$$

Consider first the scaling function $\phi_0(s)$. For small s , one obtains $\phi_0(s) = 1 - 2e^{2f_0(1)\gamma} s^{2f_0(1)} + \dots$, where $\gamma = 0.577, \dots$ is Euler's constant. But, from the definition of $\phi_0(s)$ as the Laplace transform of $f_0(x)$, one also has $\phi_0(s) = 1 - s\langle x \rangle_0 + \dots$, where $\langle x \rangle_0$ is the mean domain size (in units of the minimum domain size a) for the scaling distribution. Comparing these expansions gives $f_0(1) \leq 1/2$, with $f_0(1) = 1/2$ when the first moment of $f_0(x)$ exists, and $f_0(1) < 1/2$ when it does not. We shall primarily consider the former case, appropriate to an initial distribution with a finite first moment.

Now consider the small- s behavior of the correction-to-scaling function $\phi_1(s)$. The factor $1 - \phi_0^2(s)$ in Eq. (31) behaves as $s^{2f_0(1)}$ for $s \rightarrow 0$, i.e., as s for $f_0(1) = 1/2$. For this case, the small- s expansion of $\phi_1(s)$ contains a nonanalytic term $s^{1+\omega}$ for any $\omega > 0$ (with a $\ln s$ factor when ω is an integer). This in turn implies that the correction-to-scaling function $f_1(x)$ has the power-law tail $x^{-(2+\omega)}$. This means that if the domain-size distribution is given by the scaling distribution $f_0(x)$ plus a small perturbation with a power-law tail $x^{-(2+\omega)}$, the perturbation is *irrelevant* (i.e., decays to zero) for $\omega > 0$, and *the correction-to-scaling exponent is ω* . More generally, any initial distribution with a power-law tail $x^{-(2+\omega)}$, with $\omega > 0$, flows to the scaling distribution $f_0(x)$ with $f_0(1) = 1/2$. For $\omega < 0$, the perturbation is relevant. In this connection one should note that the scaling distributions with $f_0(1) < 1/2$ have the power-law tail $x^{-[1+2f_0(1)]}$, i.e., they decay more *slowly* than $1/x^2$. So any initial condition that falls off more quickly than one of these "special" fixed

distributions flows to the "generic" fixed distribution with $f_0(1) = 1/2$ (which may easily be shown to have an exponential tail).

We have shown that any finite correction-to-scaling exponent ω corresponds to a correction-to-scaling function with a power-law tail. This implies that corrections to scaling that decay faster than any power-law in the scaling variable x have an infinite correction to scaling exponent, i.e., that the amplitude of the correction does not have the power-law form $a^{-\omega}$ assumed in Eq. (26). To clarify this case, we construct the exact solution of Eq. (25) for an arbitrary initial condition:

$$\phi(p,a) = \tanh \left[\int_a^\infty da' P(a',a') \exp(-pa') \right]. \quad (32)$$

The arbitrary function of p that formally appears inside the argument of the tanh, as an additive integration constant, must vanish because $\phi(p,\infty) = 0$. The function $P(a,a)$ appearing in Eq. (32) is determined by the initial condition, for which $a = a_0$, through the inverse Laplace transform

$$P(a,a) = \int_C \frac{dp}{4\pi i} \exp(pa) \ln \left(\frac{1 + \phi(p,a_0)}{1 - \phi(p,a_0)} \right), \quad (33)$$

where the contour C runs parallel to the imaginary axis, to the right of any singularities of the integrand. An equivalent result has been presented in [14]. The present approach is more direct and general.

Equations (32) and (33) represent an exact closed-form solution for the full evolution from an arbitrary initial condition. For explicit results, however, one needs to be able to evaluate the Bromwich integral (33). For illustrative purposes, we consider two simple initial conditions. The first is the simple exponential distribution $P(l,0) = \mu \exp(-\mu l)$, with the Laplace transform $\phi(p,0) = \mu/(p + \mu)$ (i.e., $a_0 = 0$ here). Inserting this in Eq. (33) gives

$$P(a,a) = \frac{1}{2a} [1 - \exp(-2\mu a)]. \quad (34)$$

One sees that $P(a,a)$ approaches the scaling limit $1/2a$ exponentially fast as a function of a , i.e., faster than any power. This is in accord with our result that a power-law correction to scaling is associated with power-law tails in the initial domain-size distribution. Inserting Eq. (34) into Eq. (32), and expanding for $\mu a \gg 1$, gives

$$\begin{aligned} \phi(p,a) = & \phi_0(s) - \frac{1}{4\mu a} \exp(-2\mu a) \exp(-s) [1 - \phi_0(s)^2] \\ & + \dots, \end{aligned} \quad (35)$$

where $\phi_0(s)$ (with $s=pa$) is the scaling function. Again, the correction is exponentially small.

Our second example shows that the correction to scaling can be an oscillatory function of a . For $P(l,0) = \mu^2 l \exp(-\mu l)$, one obtains $\phi(p,0) = \mu^2/(p + \mu)^2$. Inserting this into Eq. (33) gives $P(a,a) = [1 - 2\cos(\mu a)\exp(-\mu a) + \exp(-2\mu a)]/2a$, so that the leading correction to scaling is the term involving $\cos(\mu a)$. The difference between this case and the first example is that in the former the singularities of

the function $h(p) \equiv \ln\{[1 + \phi(p,0)]/[1 - \phi(p,0)]\}$ appearing in Eq. (33) are branch points on the real axis at $p=0$ and -2μ , whereas in the latter they are branch points at $p=0$, $-(1 \pm i)\mu$ and -2μ . The leading scaling part $1/2a$ in $P(a,a)$ is associated with the singularity of $h(p)$ at $p=0$. The leading correction to scaling derives from the singularity with the largest real part (excluding $p=0$). If this singularity is off the real axis, the leading correction to scaling will be oscillatory. In all the other models considered in this paper, however, the leading correction to scaling is monotonically decreasing function of time.

V. THE OJK THEORY

The theory of Ohta, Jasnow, and Kawasaki (OJK) [2] for the pair correlation function of a nonconserved scalar field starts from the Allen-Cahn equation relating the interface velocity to its local curvature [6]. The theory is expressed in terms of a ‘‘smooth’’ auxiliary field $m(\mathbf{x},t)$ whose zeros give the positions of the interfaces between domains of the two phases. The field m obeys the diffusion equation $\partial m/\partial t = \nabla^2 m$ (we absorb the diffusion constant into the time scale). The initial conditions are taken to be Gaussian. The normalized pair correlation function of m is

$$\gamma(r,t) = \frac{\langle m(\mathbf{x},t) m(\mathbf{x} + \mathbf{r},t) \rangle}{\langle m(\mathbf{x},t)^2 \rangle}, \quad (36)$$

while the correlation function for the order-parameter field ϕ is

$$C(r,t) = \langle \text{sgn}[m(\mathbf{x},t)] \text{sgn}[m(\mathbf{x} + \mathbf{r},t)] \rangle = \frac{2}{\pi} \sin^{-1} \gamma(r,t). \quad (37)$$

Note that by using the sgn function to relate the order parameter to the auxiliary field we are working in the ‘‘thin wall’’ limit. This means that we are neglecting any corrections to scaling associated with the finite width of the domain walls, and are focusing instead on corrections deriving from the initial conditions. This is the same approach that we are using throughout this paper.

It is simplest, in the first instance, to compute the corrections to scaling associated with the function $\gamma(r,t)$. If we define $h(r,t) = \langle m(\mathbf{x},t) m(\mathbf{x} + \mathbf{r},t) \rangle$, then $\gamma(r,t) = h(r,t)/h(0,t)$. From the diffusion equation for m , one obtains immediately $(1/2)\partial_t h = \nabla^2 h$, giving $(1/2)\partial_t \gamma = \nabla^2 \gamma + \alpha(t)\gamma$, where $\alpha(t) = -[\partial_t \ln h(0,t)]/2$. Since h satisfies a diffusion equation, we know that for a short-ranged initial condition, peaked around $r=0$, $h(0,t) \sim t^{-d/2}$ asymptotically, giving $\alpha(t) \rightarrow d/4t$ for large t . It is convenient, however, to incorporate corrections to scaling in $L(t)$ through the requirement that $\alpha(t) = \lambda/2L^2$ exactly, i.e., $(1/2)\partial_t \gamma = \nabla^2 \gamma + (\lambda/2L^2)\gamma$. Choosing the scale of L such that $L \rightarrow t^{1/2}$ asymptotically then fixes $\lambda = d/2$, as in the large- n theory. Writing $\gamma(r,t) = \gamma_0(r/L) + L^{-\omega} \gamma_1(r/L)$, and $\dot{L} = 1/2L + b/L^{1+\omega}$, as usual, substituting into the equation for γ , and equating leading and next-to-leading powers of L , gives

$$\gamma_0'' + \left(\frac{d-1}{x} + \frac{x}{4} \right) \gamma_0' + \frac{d}{4} \gamma_0 = 0, \quad (38)$$

$$\gamma_1'' + \left(\frac{d-1}{x} + \frac{x}{4} \right) \gamma_1' + \left(\frac{d+\omega}{4} \right) \gamma_1 + \frac{b}{2} x \gamma_0' = 0. \quad (39)$$

In fact these equations are identical to Eqs. (19) and (20) of the large- n theory, with the same boundary conditions, and the results for γ_0 and γ_1 can be simply read off:

$$\gamma_0(x) = \exp(-x^2/8), \quad (40)$$

$$\gamma_1(x) = [bx^4/32(d+2)] \exp(-x^2/8). \quad (41)$$

The correction-to-scaling exponent is $\omega=4$, as in the large- n theory.

The order-parameter correlation function $C(r,t)$ has the expansion $C(r,t) = f_0(r/L) + L^{-\omega} f_1(r/L) + \dots$. The functions $f_0(x)$ and $f_1(x)$ follow immediately from Eqs. (37), (40), and (41):

$$f_0(x) = \frac{2}{\pi} \sin^{-1} \gamma_0(x), \quad (42)$$

$$f_1(x) = \frac{2}{\pi} \frac{\gamma_1(x)}{[1 - \gamma_0^2(x)]^{1/2}}. \quad (43)$$

Note that $f_1(x) \sim x^3$ for small x , so that the linear term in x from f_0 is not modified—our definition of L has ensured that areal density of domain walls, and therefore the energy, varies as $1/L$ exactly.

VI. THE MAZENKO THEORY

An alternative ‘‘Gaussian closure’’ theory to that of OJK has been proposed by Mazenko [3]. For nonconserved scalar fields, the pair correlation function $C(r,t)$ satisfies the closed equation

$$\frac{1}{2} \frac{\partial C}{\partial t} = \nabla^2 C + \frac{1}{\pi S_0(t)} \tan\left(\frac{\pi}{2} C\right). \quad (44)$$

The function $S_0(t)$ is defined as $\langle m(\mathbf{r},t)^2 \rangle$, where m is a Gaussian auxiliary field as before. For the present purposes, however, it is sufficient to note that S_0 has dimensions $(\text{length})^2$. In fact, it is convenient to define the coarsening length scale $L(t)$ by $S_0 = L^2/\lambda$, where λ is a constant whose value is fixed by physical requirements [3]. This definition of L is in accord with our previous definitions, as we shall see.

Writing $S_0 = L^2/\lambda$ in Eq. (44), setting $C(r,t) = f_0(r/L) + L^{-\omega} f_1(r/L) + \dots$, $dL/dt = 1/2L + b/L^{1+\omega} + \dots$, and equating leading and next-to-leading powers of L in the usual way gives the following equations for the functions $f_0(x)$ and $f_1(x)$:

$$f_0'' + \left(\frac{d-1}{x} + \frac{x}{4} \right) f_0' + \frac{\lambda}{\pi} \tan\left(\frac{\pi}{2} f_0\right) = 0, \quad (45)$$

$$f_1'' + \left(\frac{d-1}{x} + \frac{x}{4} \right) f_1' + \frac{\lambda}{2} \sec^2\left(\frac{\pi}{2} f_0\right) f_1 + \frac{\omega}{4} f_1 + \frac{b}{2} x f_0' = 0. \quad (46)$$

Equation (45) is to be solved with boundary conditions $f_0(0) = 1$, $f_0'(0) = -(1/\pi)[2\lambda/(d-1)]^{1/2}$, the latter follow-

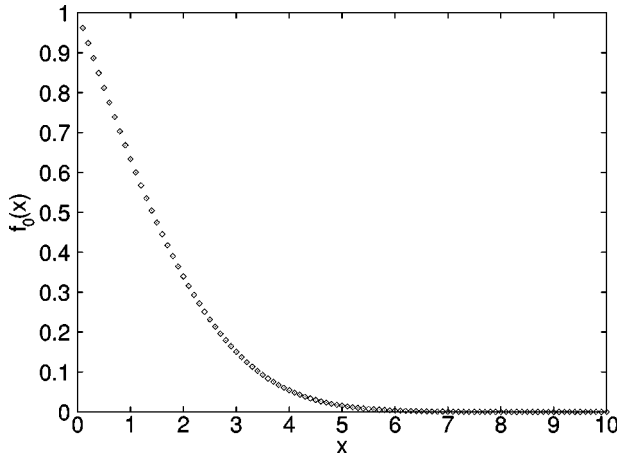


FIG. 1. The scaling function $f_0(x)$ in the Mazenko theory for $d=2$.

ing from a small- x analysis of the equation. The parameter λ is determined as follows [3]. For large x , Eq. (45) reduces to the linear equation $f_0'' + [(d-1)/x + x/4]f_0' + (\lambda/2)f_0 = 0$. This equation has the same form as the large- n equation (19), and the two linearly independent large- x solutions have the large- x forms $x^{-2\lambda}$ and $\sim \exp(-x^2/8)$ discussed in Sec. III. If the equation is integrated forward from $x=0$, for general λ a linear combination of the two large- x solutions will be obtained. But a power-law decay is unphysical if the initial conditions contain only short-range spatial correlations. The parameter λ is fixed by the requirement that this unphysical power-law decay be absent. Imposing this condition through a numerical solution of Eq. (45) gives $\lambda = 0.711\,277$ for $d=2$, and $\lambda = 1.327\,411$ for $d=3$ (correct to the number of figures given). The exponent $\bar{\lambda}$, which describes the decay of the autocorrelation function via $\langle \phi(\mathbf{x}, t) \phi(\mathbf{x}, 0) \rangle \sim L(t)^{-\bar{\lambda}}$, is given by $\bar{\lambda} = d - \lambda$ within this theory [4]. For $d \rightarrow \infty$, the OJK solution is recovered and $\lambda \rightarrow d/2$.

The correction to scaling ω is determined in a similar way from Eq. (46). The boundary conditions on this equation are $f_1(0) = 0 = f_1'(0)$. For large x , the homogeneous part of this equation (i.e., without the final term) reduces to the homogeneous part of the equivalent large- n equation (20). The two linearly independent large- x solutions decay as $\sim \exp(-x^2/8)$ and $\sim x^{-2\lambda-\omega}$. The exponent ω is determined by the condition that the power-law decaying term is absent from the large- x solution. Implementing this condition numerically gives $\omega = 3.8836$ for $d=2$ and $\omega = 3.9030$ for $d=3$. For $d \rightarrow \infty$, the OJK result $\omega = 4$ is recovered.

Figures 1 and 2 show the scaling and correction-to-scaling functions for $d=2$ (those for $d=3$ are very similar). The *amplitude* of the correction to scaling function is fixed by the constant b in equation (46). The value $b = 2$ was used in Fig. 2.

Note that, within the Mazenko approach, the exponent ω is *nontrivial*. Indeed in this theory ω is on the same footing as $\bar{\lambda}$, which is known to be nontrivial in general. This suggests that, like $\bar{\lambda}$, the correction-to-scaling exponent ω is in general a nontrivial exponent of phase-ordering kinetics.

VII. CONCLUSION

An understanding of the corrections to scaling is important in analyzing data from experiments or simulations. In

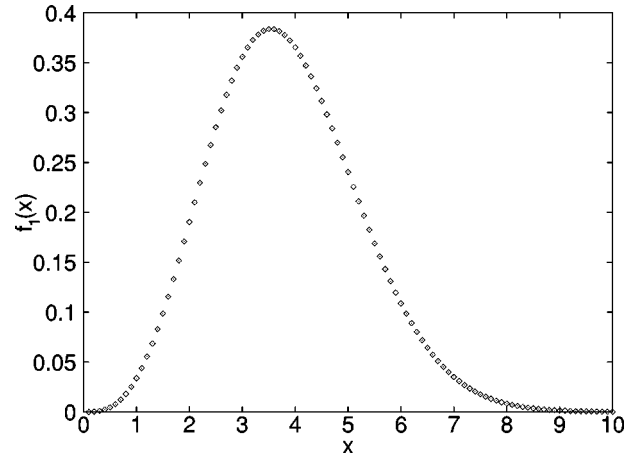


FIG. 2. The correction-to-scaling function $f_1(x)$ in the Mazenko theory for $d=2$.

this paper we have computed the correction-to-scaling exponents ω , and the corresponding correction-to-scaling functions, for a number of models of phase-ordering dynamics. For simplicity we have focused on the correction to scaling associated with the approach of the order-parameter morphology to its scaling form, i.e., the correction arising from a nonscaling initial condition, and have suppressed contributions associated with, for example, the finite thickness of the domain walls by working in the thin-wall limit.

In simple soluble models such as the 1D Glauber model, the $n = \infty$ model, and the OJK theory, the exponent ω takes an integer value, $\omega = 4$. Within the Mazenko theory, however, ω takes nontrivial values, suggesting that this exponent is, in general, a *new nontrivial exponent* of phase-ordering kinetics. The 1D TDGL equation is anomalous in that corrections to scaling vanish exponentially fast as a function of the smallest domain size.

It is important to note that the values of ω computed in this paper correspond to a special, though natural, definition of the domain scale L through the mean energy density. Specifically the energy density is defined to be exactly $1/L$ (up to an overall constant) for the scalar models, i.e., the areal density of domain walls is proportional to $1/L$, except for the 1D TDGL equation where the scale length was conveniently chosen to be the size of the smallest domain. For the large- n nonlinear sigma model, the energy density is defined to be exactly $1/L^2$, again up to an overall constant. These definitions of L are optimal in that they minimize the corrections to scaling, expressed in terms of L , i.e. they maximize ω .

In the present paper we have considered systems with nonconserved order parameter only. In future work we hope to discuss corrections to scaling in systems with conserved order parameter.

ACKNOWLEDGMENTS

This work was supported by EPSRC under Grant No. GR/K53208 (A.B. and S.C.), and by the Commonwealth Scholarship Commission (N.R.). We thank I. Ispolatov for bringing Ref. [14] to our attention.

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