PHYSICAL REVIEW E VOLUME 47, NUMBER 1 JANUARY 1993

Topological defects, correlation functions, and power-law tails in phase-ordering kinetics

A. J. Bray
Department of Theoretical Physics, The University, Manchester M13 9PL, United Kingdom
(Received 16 June 1992)

The correlation functions C_ϕ and C_{ϕ^2}, associated with the order-parameter field $\vec{\phi}(\mathbf{r},t)$ and its square, respectively, are discussed using heuristic arguments and an approximate analytical approach. Topological defects (walls, strings, monopoles) in the field, seeded by a quench from the high- to the low-temperature phase, lead to singular short-distance behavior in the scaling functions, and power-law tails in the corresponding structure factors. For superfluid helium, the structure factor $S_{\phi^2}(\mathbf{k},t)$ is measurable in principle using small-angle scattering (whereas S_ϕ is inaccessible). It is predicted to exhibit a power-law tail, $\sim[a^4/L(t)^2](\ln ka)^2/k$, where $L(t)$ is the characteristic scale at time t after the quench and a is the core size of a vortex line. Correlation functions for the defect density are also discussed.

PACS number(s): 64.60.Cn, 64.60.My

I. INTRODUCTION

Traditionally, the major questions of interest in the theory of phase-ordering dynamics have been the nature of the growth law for the characteristic scale $L(t)$ and the form of the scaling function $f(x)$ for the two-point correlation function of the order parameter field ϕ[1]. For a scalar field, one has $L(t)\sim t^{1/2}$ or $t^{1/3}$ for nonconserved and conserved fields, respectively, and, according to the scaling hypothesis, the two-point correlation function has the scaling form [1]

$$C_\phi(\mathbf{r},t)\equiv\langle\phi(\mathbf{x},t)\phi(\mathbf{x}+\mathbf{r},t)\rangle=f_\phi(r/L(t)) \ . \qquad (1)$$

Although the validity of the scaling hypothesis has not been rigorously established, it is supported by a wealth of experimental and simulational data.

In contrast to C_ϕ, the correlation function for the square of the field

$$\begin{aligned}C_{\phi^2}(\mathbf{r},t)&\equiv\langle\phi^2(\mathbf{x},t)\phi^2(\mathbf{x}+\mathbf{r},t)\rangle_c\\&\equiv\langle\phi^2(\mathbf{x},t)\phi^2(\mathbf{x}+\mathbf{r},t)\rangle\\&\quad-\langle\phi^2(\mathbf{x},t)\rangle\langle\phi^2(\mathbf{x}+\mathbf{r},t)\rangle\end{aligned} \qquad (2)$$

has received little attention. The emphasis on C_ϕ is readily understandable: C_ϕ [in fact its spatial Fourier transform, the structure factor $S_\phi(\mathbf{k},t)$] is directly measurable via small-angle scattering experiments. Fourier transforming (1) gives

$$S_\phi(\mathbf{k},t)=L(t)^d g_\phi(kL(t)) \ , \qquad (3)$$

where d is the spatial dimension.

There has been much recent interest, however, in phase ordering in systems for which the order parameter has a continuous symmetry [2–9]. Such systems include superfluid helium, superconductors, liquid crystals [6], and any system described by a vector order parameter. For superfluid helium and superconductors the order parameter is a complex scalar ψ, which does not couple to any physical probe. As a result, the usual two-point correlation function $\langle\psi^*(\mathbf{x},t)\psi(\mathbf{x}+\mathbf{r},t)\rangle$ cannot be measured. Rather, experimental probes couple to $|\psi|^2$. Since the complex field can be expressed in terms of two real fields, $\psi=\phi_1+i\phi_2$, the theory of a complex field is equivalent to an $n=2$ vector theory. Furthermore, small-angle scattering experiments then measure the Fourier transform of the correlation function C_{ϕ^2} defined by (2). It is therefore of interest to investigate the form of C_{ϕ^2}.

While the precise form of the scaling functions $f(x)$ is not known, the general features are well understood. Of particular interest is the short-distance behavior, since this is reflected in the large-k, or "tail," behavior of the structure factor. By "short" distance, we mean r in the range $a \ll r \ll L(t)$, where a is the lower limit of the scaling regime, set by the domain wall thickness, vortex core size, etc. as appropriate. For a scalar field, the sharpness of the domain walls [whose thickness a remains fixed as $L(t)\to\infty$] leads to the small-x behavior [where $x=r/L(t)$] $f_\phi(x)=1-\text{const}\times x+\cdots$. This in turn implies the power-law tail, $S_\phi(k,t)\sim L(t)^{-1}k^{-(d+1)}$, in the structure factor for $k(L)t\gg1$ (but $ka\ll1$), the celebrated "Porod's law" [10]. Very recently this result has been generalized to vector fields, with the result [7]

$$S_\phi(k,t)\sim L(t)^{-n}k^{-(d+n)} \ , \qquad (4)$$

for $kL(t)\gg1$. Numerical simulation results [4,5,11] are consistent with Eq. (4). We will show below how this result follows very simply from the idea that the relevant topological defects in the field are responsible for the tail.

The principal new idea in the present paper is that the correlation function $C_{\phi^2}(\mathbf{r},t)$ also has interesting short-distance behavior and is, in fact, more singular at short distance than C_ϕ. In consequence, its Fourier transform $S_{\phi^2}(\mathbf{k},t)$ has a more pronounced power-law tail (i.e., with a smaller power) than does S_ϕ. To be precise, we find

$$S_{\phi^2}(\mathbf{k},t)\sim\begin{cases}a^2L(t)^{-1}k^{-(d-1)} & (n=1) \qquad (5)\\ a^4L(t)^{-2}\ln^2(ka)k^{-(d-2)} & (n=2) \qquad (6)\\ a^4L(t)^{-n}k^{-(d+n-4)} & (n>2) \qquad (7)\end{cases}$$

for $kL(t) \gg 1$, provided $n \le d$ so that the relevant topological defects are present in the system. It will be interesting to test these predictions through experiments and numerical simulations.

A related question concerns defect-defect correlations during phase ordering. If $\rho(\mathbf{r},t)$ is the density of domain walls, vortices, strings, etc., as appropriate, then one can define the density-density correlation function

$$C_\rho(\mathbf{r},t) = \langle \rho(\mathbf{x},t)\rho(\mathbf{x}+\mathbf{r},t)\rangle_c \ , \tag{8}$$

where $\langle\ \rangle_c$ indicates a "connected" correlation function, as in (2). Related correlation functions, in which the defect "charges" (or orientations, for extended defects) are incorporated in the definition of the density, have recently been discussed by Liu and Mazenko [12]. Below we will show that for scalar fields C_ρ is closely related to C_{ϕ^2}. We will also discuss the form of C_ρ for vector fields.

The paper is organized as follows. Heuristic arguments for the tail behavior given by (4)–(7) are presented in Sec. II. An approximate analytical treatment, based on an approach originated by Mazenko [13], is given in Sec. III, and yields expressions for C_{ϕ^2} whose short-distance behavior reproduces (5)–(7). Section IV contains results for the defect correlation function C_ρ for both scalar and vector fields, and a comparison with the results of [12]. The results are discussed and summarized in Sec. V.

II. HEURISTIC ARGUMENTS

We now present the simple heuristic argument leading to Eqs. (4)–(7). To derive (4) we start from (3) and observe that, for $kL(t) \gg 1$, one is probing distances short compared to the distance $L(t)$ between topological defects. Therefore one expects the structure factor in this regime to be the sum of essentially independent contributions from different defects, or from parts of the same defect separated by more than k^{-1}. It follows that $S_\phi(\mathbf{k},t)$ should scale as the total defect density, i.e., as the "amount of defect" per unit volume. For walls ($n=1$), this is the wall area per unit volume, and scales as $L(t)^{-1}$. For vortices ($d=2=n$) or strings ($d=3, n=2$) it is the number of vortices per unit area, or the length of string per unit volume, respectively, both scaling as $L(t)^{-2}$. For monopoles ($d=3=n$), it is the number of monopoles per unit volume, and scales as $L(t)^{-3}$. In fact for general $n \le d$, the defect density scales as $L(t)^{-n}$. Requiring this factor for the t dependence of $S_\phi(\mathbf{k},t)$ when $kL(t) \gg 1$ requires the asymptotic form $g_\phi(x) \sim x^{-(d+n)}$ for $x \to \infty$ in (3), and (4) follows immediately.

A similar argument can be used to derive (5) and (7). The first step is to motivate scaling forms for C_{ϕ^2} and S_{ϕ^2} analogous to (1) and (3). To facilitate this we rewrite (2) in the form

$$C_{\phi^2}(\mathbf{r},t) = \langle [1-\phi^2(1)][1-\phi^2(2)]\rangle - \langle [1-\phi^2(1)]\rangle\langle [1-\phi^2(2)]\rangle \ , \tag{9}$$

where we have introduced the shorthand "1" for $(\mathbf{r}_1,t)$, etc., and now $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$.

Consider first a scalar field. We can estimate $\langle(1-\phi^2)\rangle$ by observing that $(1-\phi^2)$ vanishes except inside domain walls, which occupy a fraction of order $a/L(t)$ of space, where a is a measure of the wall thickness. This gives $\langle(1-\phi^2)\rangle \sim a/L(t)$. Therefore the anticipated scaling form for (9) is

$$C_{\phi^2}(\mathbf{r},t) = a^2 L(t)^{-2} f_{\phi^2}(r/L(t)) \ , \tag{10}$$

while the corresponding form for the structure factor is

$$S_{\phi^2}(\mathbf{k},t) = a^2 L(t)^{d-2} g_{\phi^2}(kL(t)) \ . \tag{11}$$

For $kL(t) \gg 1$ we again invoke the argument that S_{ϕ^2} should scale as the total wall density, i.e., as $1/L(t)$. This requires $g_{\phi^2}(x) \sim x^{-(d-1)}$ for $x \to \infty$ in (11), which in turn implies (5).

For a vector theory, there is no well-defined "size" of a defect core: instead $1-\phi^2 \sim a^2/r^2$ for $r \gg a$, where r is the distance from the defect (in the scalar theory, $1-\phi^2$ vanishes exponentially with r/a). Since the defect density is of order $L(t)^{-n}$, we estimate

$$\langle(1-\phi^2)\rangle \sim L(t)^{-n}\int_a^{L(t)} d^n r (a/r)^2 \sim \begin{cases} a^2/L(t)^2, & n>2 \\ a^2[(\ln L(t)]/L(t)^2, & n=2 \ , \end{cases} \tag{12}$$

where the integration is over the n-dimensional subspace orthogonal to the defect, and the upper cutoff at $L(t)$ represents the limiting distance at which the defect field can be taken to be undisturbed by other defects. The case $n=2$, while of great physical interest, is complicated by the appearance of the logarithm in (12), and its discussion will be deferred for the moment. For $n>2$, (12) suggests the scaling forms

$$C_{\phi^2}(\mathbf{r},t) = a^4 L(t)^{-4} f_{\phi^2}(r/L(t)) \ , \tag{13}$$

$$S_{\phi^2}(\mathbf{k},t) = a^4 L(t)^{d-4} g_{\phi^2}(kL(t)) \ . \tag{14}$$

For $kL(t) \gg 1$ the argument that S_{ϕ^2} should scale as the total defect density, i.e., as $L(t)^{-n}$, requires $g_{\phi^2}(x) \sim x^{-(d+n-4)}$ for $x \to \infty$ in (13), which in turn implies (7). The scaling forms (5) and (7) will be supported by the approximate analytic treatment given below, which also yields (6) for $n=2$.

We mentioned in the Introduction that the power-law tails in k space are related to singular short-distance behavior of the scaling functions in real space. This will emerge explicitly from the following analytic treatment. For scalar fields, (5) implies the short-distance behavior $f_{\phi^2}(x) \sim 1/x$ for $x \to 0$ in (10). This also follows from the analytical treatment given below and from direct intuitive arguments.

III. ANALYTIC TREATMENT

We will take the Hamiltonian of the system to have usual Ginzburg-Landau form

$$H = \int d^d\vec{\phi}[\tfrac{1}{2}(\nabla\vec{\phi})^2 + V(\vec{\phi})] \ , \tag{15}$$

where the potential $V(\vec{\phi})$ has the standard "mexican hat" (sombrero) form, with ground-state manifold $\phi^2=1$.

The essential idea, exploited by a number of authors [7–9,12–14], is to express the field $\vec{\phi}(\mathbf{x},t)$, which varies very rapidly near defects, in terms of a "smooth" field $\vec{m}(\mathbf{x},t)$. We will follow Mazenko's suggestion [13,8,9] of defining the function $\vec{\phi}(\vec{m})$ by the equation

$$\nabla_m^2 \vec{\phi} = \frac{\partial V}{\partial \vec{\phi}} , \tag{16}$$

with boundary conditions $\vec{\phi}(0)=\vec{0}$ and $\vec{\phi}(\vec{m})\rightarrow\hat{m}$ for $|\vec{m}|\rightarrow\infty$, where $\hat{m}\equiv\vec{m}/|\vec{m}|$. Since the equilibrium field of a defect is given by $\delta H/\delta\vec{\phi}=\vec{0}=-\nabla^2\vec{\phi}+\partial V/\partial\vec{\phi}$, it is clear that, close to a defect, where the field is not significantly disturbed by neighboring defects, $\vec{m}(\mathbf{x},t)$ can be identified as the position vector to the point $\mathbf{x}$ from the defect (for point defects) or from the nearest part of the defect (for extended defects). This identification will be exploited in Sec. IV to simplify the calculation of defect correlation functions. The key assumption of Mazenko's approach is that the field $\vec{m}(\mathbf{x},t)$ can be taken to have a Gaussian distribution. It should be emphasized that this is an uncontrolled approximation, although there are indications [15] that it may become valid in the limit $d\rightarrow\infty$. Since we compute correlation functions involving only two different space points, we require only the joint distribution function $P(\vec{m}(1),\vec{m}(2))$ of the fields at points "1" and "2." It is given by [7–9]

$$P(\vec{m}(1),\vec{m}(2))=\frac{1}{N^n}\exp\left\{-\frac{1}{2(1-\gamma^2)}\left[\frac{\vec{m}(1)^2}{S_0(1)}+\frac{\vec{m}(2)^2}{S_0(2)}-\frac{2\gamma\vec{m}(1)\cdot\vec{m}(2)}{[S_0(1)S_0(2)]^{1/2}}\right]\right\} , \tag{17}$$

where

$$S_0(1)=\langle m(1)^2\rangle,\quad S_0(2)=\langle m(2)^2\rangle ,$$
$$\gamma=\frac{\langle m(1)m(2)\rangle}{[S_0(1)S_0(2)]^{1/2}} , \tag{18}$$
$$N=\frac{1}{2\pi[(1-\gamma^2)S_0(1)S_0(2)]^{1/2}} ,$$

where $m(1),m(2)$ refer to a given Cartesian component of the vectors $\vec{m}(1)$, $\vec{m}(2)$, the different components of a Gaussian field being independent. In this paper we will be exclusively interested in equal-time correlations (although the different-time results are a trivial extension), so we will set $S_0(1)=S_0(2)=S_0$. Furthermore, the identification of $\vec{m}$ as a spatial position vector near defects leads to the scaling [8,9,13] $S_0\equiv\langle m^2\rangle\sim L(t)^2$. The dependence on the spatial separation r of the points 1 and 2 enters through γ, which is the normalized correlation function for one components of the field $\vec{m}$. In particular, $\gamma=1$ for $r=0$, and $\gamma=0$ for $r=\infty$.

Mazenko has shown [13], in the context of the scalar theory, how to exploit the transformation from ϕ to m, and the distribution (17), to evaluate the correlation function C_ϕ. Essentially, one uses the fact that, as far as scaling properties are concerned, one can use $\phi\simeq\mathrm{sgn}(m)$, which is valid almost everywhere at late times. Then one obtains, from (17), $C_\phi=(2/\pi)\sin^{-1}(\gamma)$. The generalization to vector fields uses $\vec{\phi}\simeq\hat{m}$ at late times to obtain [7–9]

$$C_\phi=\frac{n\gamma}{2\pi}\left[B\left[\frac{n+1}{2},\frac{1}{2}\right]\right]^2 F\left[\frac{1}{2},\frac{1}{2};\frac{n+2}{2};\gamma^2\right] , \tag{19}$$

where $B(x,y)$ is the beta function and $F(a,b;c;z)$ the hypergeometric function. To determine γ requires a specific equation of motion. For the time-dependent Ginzburg-Landau (TDGL) equation, $\partial\vec{\phi}/\partial t=-\delta H/\delta\vec{\phi}$, the Gaussian property of $\vec{m}$ can be exploited to determine a closed equation for the function $\gamma(\mathbf{r},t)$. Within the simpler theory of Ohta, Jasnow, and Kawasaki (OJK) [14], and its generalization to vector fields [7], γ is simply given by $\gamma=\exp(-r^2/2L^2)$, with $L\sim t^{1/2}$. As far as the *short-distance* properties of C_ϕ are concerned, the important point is that $1-\gamma^2\sim r^2/L^2$ for $r\ll L$: the leading short-distance singularities in C_ϕ follow from the singular (for $\gamma\rightarrow 1$) dependence of C_ϕ on γ implied by (19) [7–9].

We now apply these same ideas to the calculation of C_{ϕ^2}.

A. Scalar fields

In terms of the m field one has

$$\langle[1-\phi^2(1)][1-\phi^2(2)]\rangle=\int dm(1)\int dm(2)P(m(1),m(2))[1-\phi^2(m(1))][1-\phi^2(m(2))] . \tag{20}$$

The function $\phi(m)$ is a sigmoid function which approaches ±1 exponentially fast for $m\rightarrow\pm\infty$ [e.g., for the ϕ^4 potential, $V(\phi)=(1-\phi^2)^2/4$, one has $\phi(m)=\tanh(m/\sqrt{2})$], with a "width" equal to the domain-wall width a [from (16), $\phi(m)$ is just the domain-wall profile function]. On the other hand, the probability distribution $P(m(1),m(2))$ varies slowly as a function of its arguments, on the scale of the domain length $L(t)$. Therefore this latter factor may be taken outside the integral in (20), and evaluated at $m(1)=0=m(2)$, because the $[1-\phi^2(m)]$ factors converge the integrals. This gives, in the scaling limit,

$$\langle[1-\phi^2(1)][1-\phi^2(2)]\rangle=a^2P(0,0)$$
$$=\mathrm{const}\times\frac{a^2}{L(t)^2}\times\frac{1}{(1-\gamma^2)^{1/2}} , \tag{21}$$

where we used (17) (with $n=1$) for $P(0,0)$. The factor a^2 in (21) arises from the convenient definition $\int_{-\infty}^{\infty} dm[1-\phi^2(m)]=a$ for the width of a wall. The factor L^{-2} comes from the factor S_0^{-1} in $P(0,0)$, since $S_0 \sim L(t)^2$. The second term in (9) is generated by setting $\gamma=0$ in (21), which corresponds to the limit $r/L \to \infty$. This gives the connected correlation function (9) as

$$C_{\phi^2}(\mathbf{r},t)=\text{const}\times\frac{a^2}{L(t)^2}\left[\frac{1}{(1-\gamma^2)^{1/2}}-1\right] . \tag{22}$$

For $r \ll L$, $1-\gamma^2 \sim r^2/L^2$ gives

$$C_{\phi^2}(\mathbf{r},t)\sim\frac{a^2}{L(t)r}, \quad a \ll r \ll L(t) . \tag{23}$$

Fourier transforming this result gives $S_{\phi^2}(\mathbf{k},t) \sim a^2/L(t)k^{d-1}$ for $kL(t) \gg 1$, which is (5). A heuristic derivation of (23) will be given below.

B. Vector fields, $n>2$

The analog of (19) for vector fields can be written down immediately, by letting $\phi \to \vec{\phi}$ and $m \to \vec{m}$ everywhere. The crucial difference now, however, is that $\vec{\phi}^2(\vec{m})$ no longer approaches unity exponential fast for $|\vec{m}| \to \infty$, but as a power law [8]:

$$1-\vec{\phi}^2(\vec{m}) \simeq a^2/|\vec{m}^2|, \quad |\vec{m}^2| \to \infty , \tag{24}$$

where (24) can be taken as a convenient definition of the "core size" a for a defect in a vector field. The result (24) can be derived explicitly by inserting the radially symmetric solution $\vec{\phi}(\vec{m})=\hat{m}\phi(|\vec{m}|)$ into (16) and solving for the asymptotic behavior of the profile function $\phi(x)$ (see, e.g., [8]). Inserting (24) into (20) gives

$$\langle[1-\vec{\phi}^2(1)][1-\vec{\phi}^2(2)]\rangle=a^4\int d\vec{m}(1)\int d\vec{m}(2)P(\vec{m}(1),\vec{m}(2))|\vec{m}(1)|^{-2}|\vec{m}(2)|^{-2} . \tag{25}$$

To justify the use of the asymptotic form (24) in (25) we have to argue that the $\vec{m}$ integrals are dominated by values of $|\vec{m}(1)$ and $|\vec{m}(2)|$ that are large compared to the core size a. However, this is clearly so, because (in contrast to the scalar theory) the convergence of the integrals at large $|\vec{m}(1)|$, $|\vec{m}(2)|$ is controlled by the factor $P(\vec{m}(1),\vec{m}(2))$. This varies with $|\vec{m}(1)|,|\vec{m}(2)|$ on the scale of the characteristic length $L(t)$, which is asymptotically much greater than a.

The case $n=2$ is special, because the integral (25) is then divergent for small $|\vec{m}(1)|,|\vec{m}(2)|$, and it is no longer permissible to use (24) in the integrand. We will return to this interesting case below.

For $n>2$, the integral (25), with $P(\vec{m}(1),\vec{m}(2))$ given by (17), may be evaluated by standard techniques similar to those employed in the evaluation of C_ϕ in [7–9]. In short, one employs the integral representation $|\vec{m}(i)|^{-2}=\int_0^\infty du_i \exp[-u_i\vec{m}(i)^2]$ $(i=1,2)$, carries out the Gaussian integrals over $\vec{m}(1),\vec{m}(2)$, before evaluating the final integrals over the auxiliary variables, u_1,u_2. The result is

$$\langle[1-\vec{\phi}^2(1)][1-\vec{\phi}^2(2)]\rangle=\frac{a^4}{S_0^2}\frac{1}{(n-2)^2}F(1,1;n/2;\gamma^2) . \tag{26}$$

Using once more $S_0 \sim L^2 \sim t$, and subtracting the $\gamma=0$ value (corresponding to $r=\infty$) to generate the connected correlation function, we obtain the final result

$$C_{\phi^2}(\mathbf{r},t)=\text{const}\times\frac{a^4}{L(t)^4}\frac{1}{(n-2)^2}\{F(1,1;n/2;\gamma^2)-1\} . \tag{27}$$

For the special case $n=3$, the hypergeometric function simplifies to $F(1,1;3/2;\gamma^2)=\sin^{-1}(\gamma)/\gamma(1-\gamma^2)^{1/2}$.

In this paper we are especially interested in the behavior of the Fourier transform $S_{\phi^2}(\mathbf{k},t)$ at large kL. This is related to the short-distance behavior of the real-space scaling function. For example, for $n=3$ one obtains, for $\gamma \to 1$,

$$C_{\phi^2}(\mathbf{r},t)\sim(a/L)^4(1-\gamma^2)^{-1/2}\sim(a/L)^4(L/r) , \qquad a \ll r \ll L \quad (n=3) . \tag{28}$$

For arbitrary $n>2$ this generalizes to

$$C_{\phi^2}(\mathbf{r},t)\sim\begin{cases}(a/L)^4(1-\gamma^2)^{(n-4)/2}, & 2<n<4\\ -(a/L)^4\ln(1-\gamma^2), & n=4\\ (\text{regular terms})+(1-\gamma^2)^{(n-4)/2}\times(\text{regular terms}), & n>4 .\end{cases} \tag{29}$$

For even integers n, where the factor $(1-\gamma^2)^{(n-4)/2}$ becomes regular at $\gamma=1$, an additional logarithmic factor $\ln(1-\gamma^2)$ appears, as shown explicitly in (29) for $n=4$.

In Fourier space, $(1-\gamma^2)\sim r^2/L^2$ for $r \ll L$ implies, for all $n>2$, the power-law tail

$$S_{\phi^2}(\mathbf{k},t)\sim a^4L(t)^{-n}k^{-(d+n-4)} \tag{30}$$

in the structure factor, in agreement with (7). The factor L^{-n} is in accord with our physical argument that the structure factor should be proportional to the defect density.

C. Vector fields, $n=2$

For this special case, (25) can no longer be used, as the integrals diverge (logarithmically) at small $|\vec{m}|$. To logarithmic accuracy, we can simply cut off the divergence at the core size a. A more sophisticated approach would employ a "soft cutoff," e.g., one could replace the factors $|\vec{m}|^{-2}$ in (25) by $(\vec{m}^2+a^2)^{-1}$ At the level of the leading logarithms, however, the result is independent of the way the cutoff is introduced. The analog of (26), derived in the Appendix, is

$$\langle[1-\vec{\phi}^2(1)][1-\vec{\phi}^2(2)]\rangle = \text{const}\times\left[\frac{a}{L}\right]^4 \frac{\ln^2\{(L/a)^2(1-\gamma^2)\}}{1-\gamma^2} . \quad (31)$$

The connected correlation function is obtained, as usual, by subtracting the $\gamma=0$ value to give

$$C_{\phi^2}(\mathbf{r},t)=\text{const}\times\left[\frac{a}{L}\right]^4\left\{\frac{\ln^2\{(L/a)^2(1-\gamma^2)\}}{1-\gamma^2} - \ln^2\{(L/a)^2\}\right\} . \quad (32)$$

Note that this does not have a conventional scaling form.

In the "short-distance" limit of interest, we use $(1-\gamma^2)\sim r^2/L^2$ once more to obtain

$$C_{\phi^2}(\mathbf{r},t)\sim\text{const}\times\frac{a^4}{L(t)^2}\frac{\ln^2(r/a)}{r^2} . \quad (33)$$

In k space this result takes the form

$$S_{\phi^2}(\mathbf{k},t)\sim\frac{a^4}{L^2}\frac{\ln^2(ka)}{k^{d-2}} \quad (34)$$

provided $d>2$. For $d=2$, one obtains

$$S_{\phi^2}(\mathbf{k},t)\sim-\frac{a^4}{L^2}\ln^3(ka) \quad (d=2) . \quad (35)$$

We emphasize that these results hold only in the scaling regime, defined by $ka \ll 1 \ll L/a$, in the limt $kL\to\infty$.

IV. DEFECT CORRELATION FUNCTIONS

Defect correlation functions have recently been discussed in detail by Liu and Mazenko (LM) [12]. In this section we present a simpler and more general derivation of their result for scalar fields, and obtain some additional results, for scalar and vector fields, by making a physically motivated simplification.

A. Scalar fields

For scalar fields one can define a local domain-wall density

$$\rho(\mathbf{r},t)=\delta(m(\mathbf{r},t))|\nabla m(\mathbf{r},t)| , \quad (36)$$

where $|\nabla m|$ is the Jacobian which correctly normalizes the δ function. The mean wall density scales as $1/L(t)$, with a coefficient that has been estimated in [12]. Here we investigate the correlation function

$$C_\rho(12)=\langle\rho(1)\rho(2)\rangle_c ,$$
$$=\langle\delta(m(1))\delta(m(2))|\nabla_1 m(1)|\,|\nabla_2 m(2)|\rangle_c , \quad (37)$$

in an obvious notation. In (37), the subscripts c indicate connected correlation functions as before.

As LM comment, the full correlation function (37) is difficult to evaluate because of the modulus signs on the Jacobians. Instead, they consider a different correlation function that is sensitive to the *orientations* of the walls, namely,

$$G_{ij}(12)=\langle\delta(m(1))[\partial_i^1 m(1)]\delta(m(2))[\partial_j^2 m(2)]\rangle . \quad (38)$$

LM evaluate the average by taking m to be a Gaussian random field as in Mazenko's theory of the function C_ϕ, and thereby relate G_{ij} to a second derivative of C_ϕ. Here we show that the same result may be derived more simply as follows. Consider the function

$$C_{ij}(12)=\langle[\partial_i^1\phi(1)][\partial_j^2\phi(2)]\rangle . \quad (39)$$

This can be written in terms of the field m as

$$C_{ij}(12)=\left\langle[\partial_i^1 m(1)]\left[\frac{d\phi(1)}{dm(1)}\right][\partial_j^2 m(2)]\left[\frac{d\phi(2)}{dm(2)}\right]\right\rangle . \quad (40)$$

However, the function $\phi(m)$ is a sigmoid function, varying between -1 and $+1$ as m goes from $-\infty$ to $+\infty$. Therefore $d\phi/dm$ is sharply peaked around $m=0$. In the scaling limit it may be replaced a delta function, $d\phi/dm\simeq 2\delta(m)$. This gives

$$G_{ij}(12)=(\tfrac{1}{4})C_{ij}(12)=(\tfrac{1}{4})\partial_i^1\partial_j^2 C_\phi(12) , \quad (41)$$

since the derivatives can be taken outside the average in (39). Noting that $C_\phi(12)$ depends on $\mathbf{r}_1,\mathbf{r}_2$ through $r=|\mathbf{r}_1-\mathbf{r}_2|$, the derivatives in (41) can be evaluated to yield

$$G_{ij}(\mathbf{r},t)=G_L(r,t)\hat{\mathbf{r}}_i\hat{\mathbf{r}}_j+G_T(r,t)(\delta_{ij}-\hat{\mathbf{r}}_i\hat{\mathbf{r}}_j) , \quad (42)$$

where

$$G_L(r,t)=-\frac{1}{4}\frac{\partial^2}{\partial r^2}C_\phi(r,t) ,$$
$$G_T(r,t)=-\frac{1}{4r}\frac{\partial}{\partial r}C_\phi(r,t) \quad (43)$$

are the longitudinal and transverse parts of the correlation function. These results are identical to those presented by LM. However, the derivation is more general as it does not rely on the assumption the field $m(\mathbf{r},t)$ is Gaussian.

Turning to the "full" correlation function (37), it seems that no such simple treatment is possible. Of course, C_ρ can be evaluated if one approximates m by a Gaussian random field, but the calculation is still rather involved. We suggest, instead, that the Gaussian approximation be taken at a later stage in the calculation. That the true field m, defined by Eq. (16), cannot in any case be precisely Gaussian (except for $d=\infty$) has been noted before [9]. The point is that, close to a wall, m has precisely the meaning of a coordinate normal to the wall. This means, therefore, that $|\nabla m|$, evaluated on a wall, is just unity, and may be taken outside the integral in (37). If one now makes the Gaussian approximation, the result is just

$$\langle \rho(1)\rho(2)\rangle = P(0,0) = \frac{1}{2\pi S_0}\frac{1}{(1-\gamma^2)^{1/2}} . \quad (44)$$

Subtracting off the large-distance limit to obtain the connected correlation function, and using $S_0 \simeq L(t)^2$, gives

$$C_\rho(r,t) = \text{const}\times\frac{1}{L(t)^2}\left[\frac{1}{(1-\gamma^2)^{1/2}}-1\right] . \quad (45)$$

Comparing this result with (22), we see that C_ρ has the same form (apart from a factor a^2) as C_{ϕ^2}. The reason is clear: $(1-\phi^2)$ is only nonzero within a wall and therefore measures, essentially, the wall density. The short-distance behavior of C_ρ is analogous to (23), i.e., $C_\rho \sim 1/rL(t)$. The intuitive argument for the $1/r$ dependence, promised in Sec. II, is as follows. Consider two points 1 and 2 separated by r. The probability that point 1 lies in a wall is of order $a/L(t)$, which is the volume fraction occupied by walls of thickness a. For $r \ll L(t)$, the second point 2 can only lie in the same wall. A randomly chosen point 2 a distance r from 1 will lie in the wall with a probability of order a/r, since this gives the fraction of points of radius r centered on 1 that lie in the wall, provided $r \gg a$. Therefore, the probability that both points lie in a wall is of order $a^2/rL(t)$. Since the function C_ρ is defined in terms of densities, rather than total probabilities, the factor a^2 is absent from (45).

B. Vector fields

The cases $n=d$ (point defects) and $n=d-1$ (line defects) have already been considered by LM, who calculated the defect density-density correlation functions, including the defect "charges" (point defects) or orientations (line defects) in the definition of the defect density $\rho(\mathbf{r},t)$. Here we consider the "full" density-density correlation functions, defining the density at point 1 as

$$\rho(1) = \delta(\vec{m}(1))|J(1)| , \quad (46)$$

where J is the Jacobian [of the transformation from the coordinate $\mathbf{r}$ to the field $\vec{m}(\mathbf{r})$] required to correctly normalize the δ function. The corresponding correlation function $C_\rho(12) = \langle\rho(1)\rho(2)\rangle_c$ is readily calculated for any $n \le d$ by using the same procedure as for the scalar theory. This means treating the Jacobian *exactly,* by recognizing that the identification of $\vec{m}$, close to a defect, as a position vector in the plane normal to the defect (or a position vector *from* the defect for point defects), means that $|J|=1$ exactly, at defects. To show this explicitly, one simply sets up an orthonormal coordinate system at each point of the defect structure, with the n components of $\vec{m}$ serving as coordinate axes normal to the defect, and another $d-n$ axes lying in the defect. Since $|J|=1$ at a defect, the Jacobian factor can be dropped from (46), to give the remarkably simple result

$$\begin{aligned}\langle\rho(1)\rho(2)\rangle_c &= \langle\delta(\vec{m}(1))\delta(\vec{m}(2))\rangle_c\\ &= P(0,0)(\gamma) - P(0,0)(0)\\ &= \left[\frac{1}{2\pi S_0}\right]^n\left\{\frac{1}{(1-\gamma^2)^{n/2}}-1\right\} . \end{aligned} \quad (47)$$

Only at the final stage has the Gaussian approximation (17) been used.

The short-distance behavior follows from $1-\gamma^2 \sim r^2/L^2$ for $r \ll L$. Inserting also $S_0 \sim L^2$ gives

$$C_\rho(\mathbf{r},t) \sim (Lr)^{-n}, \quad r \ll L , \quad (48)$$

a simple generalization of the result for scalar fields. Again this form is easy to understand intuitively, at least for extended defects. Consider choosing points 1 and 2 a distance $r \ll L$ apart. The probability that point 1 lies in a defect scales as L^{-n}. The dominant contribution to C_ρ for $r \ll L$ arises from cases where point 2 lies in the *same* defect. The fraction of points distant r from 1 which satisfy this condition scales as r^{-n}. This gives $C_\rho \sim (Lr)^{-n}$ for $r \ll L$. Essentially the same argument has been given by Mondello and Goldenfeld (MG) for the special case $d=3$, $n=2$, and their numerical simulation results confirm the prediction (48) for this case [5]. Of course, this argument does not apply to *point* defects. The prediction (48) is presumably spurious for point defects, an artifact of the Gaussian approximation used for $\vec{m}$.

C. Comparison with simulation data

A detailed comparison of (47) with the simulation results of MG [5] for $d=3$, $n=2$ is also possible. MG plot the string-string correlation function $\Gamma_{SS}(12) = \langle\rho(1)\rho(2)\rangle/\langle\rho\rangle^2$, which is normalized to unity at large separations. Equation (47) gives $\Gamma_{SS}=(1-\gamma^2)^{-1}$. The "OJK" expression [7–9] $\gamma=\exp(-r^2/8t)$ can be rewritten in terms of $r_{1/2}(t)$, the scale at which $C_\phi=\frac{1}{2}$, as $\gamma \simeq \exp(-r^2/2r_{1/2}^2)$ (since $r_{1/2}\simeq 2.0t^{1/2}$ in the OJK theory [9]). MG, on the other hand, use $r/d(t)$ as scaling variable, where $d(t)$ is another measure of the scaling length, defined by $\langle\rho\rangle = d(t)^{-2}$. MG find (as expected, if scaling is true) that $r_{1/2}(t)$ and $d(t)$ grow in the same way [16], with $d \simeq 1.4 r_{1/2}$. Therefore γ can be written as $\gamma \simeq \exp(-0.98r^2/d^2)$, giving $\Gamma_{SS} \simeq \{1-\exp(-1.96r^2/d^2)\}^{-1}$. This expression fits well the general functional form of the data. However, a quantitative fit requires that the factor 1.96 be replaced by a much larger number, around 4.6. (Using the "Mazenko" result for γ [8,9] instead of the simple OJK form makes no appreciable difference to the fit.) This is another indication of the limitations of the Gaussian approximation, especially at short distances which dominate the fit to Γ_{SS}.

It is interesting that the ratio $d(t)/r_{1/2}(t)$ can also be determined directly from the theory. First of all, $\langle\rho\rangle$ can be read off from (47) as $\langle\rho\rangle = (2\pi S_0)^{-1}$ [or, for general n, $\langle\rho\rangle=(2\pi S_0)^{-n/2}$] since the prefactor in (47) is just $\langle\rho\rangle^2$. Next, allowing for the factor of $\sqrt{2}$ difference in the definition of $\vec{m}$ [via (16)] between this paper and [9], $S_0(t)$ can be written as $S_0=2t/\lambda$, where [8,9] λ is the exponent related to two-time correlations. This gives $\langle\rho\rangle=\lambda/4\pi t$, and $d(t)=(4\pi t/\lambda)^{1/2}$. Now using, as before, $r_{1/2}\simeq 2.0t^{1/2}$, gives the ratio $d(t)/r_{1/2}(t)\simeq(\pi/\lambda)^{1/2}$. Using the OJK value [8,9] $\lambda=d/2$ gives $d(t)/r_{1/2}\simeq 1.45$ for $d=3$, quite close to the value determined numerically ($\simeq 1.38$ [17]). Using the value from the Mazenko theory [8,9], $\lambda\simeq 1.38$, would give $d/r_{1/2}\simeq 1.5$. For $d=2$, the OJK value $\lambda=d/2$ gives $d(t)/r_{1/2}\simeq 1.77$, the value from the Mazenko theory, $\lambda\simeq 0.83$, gives $d(t)/r_{1/2}\simeq 1.95$, while the MG simulations [4] give $\simeq 2.0$ for this ratio [17].

It is worth noting that the average string density $\langle\rho\rangle$ can also be calculated by retaining the Jacobian $|J|$ in (46) and using the Gaussian approximation for $\vec{m}$ immediately. This approach was used in [12], and gives $\langle\rho\rangle=\lambda/6\pi t$ and $\lambda/8\pi t$ for $d=3$ and 2, respectively, smaller by factors $\frac{2}{3}$ and $\frac{1}{2}$, respectively, than our result. This leads to a ratio $d/r_{1/2}$ which is *larger* by factors $(3/2)^{1/2}\simeq 1.22$ and $\sqrt{2}$, for $d=3$ and 2, respectively, than those derived above, i.e., significantly further from the simulation results. It seems, therefore, that replacing the Jacobian in (46) by unity before invoking the Gaussian approximation for $\vec{m}$ gives more accurate results.

We end this section by stressing that dimensionless ratios like $d(t)/r_{1/2}(t)$ should be *universal* numbers—the time dependence cancels out, taking with it any unknown factor relating time scales in the theory and the simulations. Such dimensionless ratios are valuable as absolute tests of approximate theories.

V. DISCUSSION AND SUMMARY

In this paper we have discussed the form of some higher-order correlation functions in the phase-ordering dynamics of a nonconserved field. Specifically we have studied the two-point function for the square of the order parameter, C_{ϕ^2}, and the two-point correlation function for the defect density, C_ρ. We have emphasized, in particular, the *short-distance* behavior, which can usually be extracted using heuristic arguments. Inasmuch as these arguments do not depend on the details of the underlying dynamics, e.g., whether the order parameter is conserved or nonconserved, but are determined by the structure of individual defects, the short-distance results (23), (29), (33), and (48) should be valid quite generally, as should the corresponding results (5)–(7) for the tail behavior of the structure factor $S_{\phi^2}(\mathbf{k},t)$. In particular we note that S_{ϕ^2} has a more slowly decaying tail than that of the conventional structure factor S_ϕ associated with the order-parameter field itself.

These calculations have particular relevance to the ordering dynamics of superfluid ^{4}He, where the usual structure factor S_ϕ cannot be measured, even in principle. Instead, small-angle scattering experiments, e.g., light scattering, measure S_{ϕ^2}. While this is not an easy experiment, due to the very weak coupling of light to the superfluid density, resulting in a weak signal, it may still be feasible. The tail is predicted to have the form (34) (with $d=3$) for scattering from a bulk superfluid, and (35) for a film. It should be noted that these forms exhibit a much slower fall-off with momentum transfer (or scattering angle) than the corresponding results for the usual structure factor S_ϕ.

The seeding of a "vortex tangle," which subsequently coarsens, by quenching ^{4}He into the superfluid phase has been suggested [18] as an analog for the production of cosmic strings in the early universe, induced by the proposed symmetry-breaking phase transition in accordance with the Higgs-Kibble mechanism. This analogy provides an additional incentive for performing the experiment. In practice, the quench into the ordered phase could be conveniently achieved by cooling the system under pressure to just above the Λ line, then crossing the Λ line by releasing the pressure. This would be both quicker, and more convenient, than a direct temperature quench.

ACKNOWLEDGMENTS

The author has benefitted greatly from discussions with J. Filipe, K. Humayun, and J. G. Kissner. Earlier discussions with N. Turok, a helpful comment by J. Reppy, and the communication by N. Goldenfeld of some unpublished results from his simulations with M. Mondello [4,5], are also gratefully acknowledged.

APPENDIX

In this appendix the integral (20) is evaluated to leading logarithmic accuracy for $n=2$. To this end it is convenient to use (25) with an implied lower cutoff at the core size a. In practice, it is convenient to use, as before, the integral representation $|\vec{m}|^{-2}=\int_0^\infty du\,\exp(-u\vec{m}^2)$ and to introduce the cutoff as an upper cutoff on the auxiliary integrations, at $u=1/a^2$. After the change of variable $u\to u/2S_0$ one obtains

$$\langle[1-\phi^2(1)][1-\phi^2(2)]\rangle = \frac{a^4}{4S_0^2}\int_0^{2S_0/a^2}du\int_0^{2S_0/a^2}dv\,\frac{1}{1+u+v+(1-\gamma^2)uv}\ . \tag{A1}$$

The dominant contribution to the integral comes from both u and v near the upper limit. Therefore we can drop the 1 in the denominator of the integrand. Rescaling $u\to(2S_0/a^2)u$, and similarly for v, gives

$$\langle[1-\phi^2(1)][1-\phi^2(2)]\rangle = \frac{a^2}{2S_0}\int_0^1 du\int_0^1 dv\,\frac{1}{u+v+\beta uv}\ , \tag{A2}$$

where

$$\beta=(1-\gamma^2)2S_0/a^2\ . \tag{A3}$$

Recalling that $S_0\sim L^2$, we have $\beta\to\infty$ in the scaling limit. Straightforward asymptotic analysis of the integral (A2) in this limit gives

$$\langle[1-\phi^2(1)][1-\phi^2(2)]\rangle \simeq \frac{a^2}{2S_0}\frac{\ln^2\beta}{\beta} \sim \frac{a^4}{L^4}\frac{\ln^2\{(1-\gamma^2)(L/a)^2\}}{1-\gamma^2}\ , \tag{A4}$$

which is (31).

[1] For reviews see, e.g., J. D. Gunton, M. San Miguel, and P. S. Sahni, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. L. Lebowitz (Academic, New York, 1983), Vol. 8, p. 267; H. Furukawa, Adv. Phys. **34**, 703 (1985); K. Binder, Rep. Prog. Phys. **50**, 783 (1987); S. Komura, Phase Transitions **12**, 3 (1988).

[2] H. Toyoki and K. Honda, Prog. Theor. Phys. **78**, 237 (1987); H. Toyoki, Phys. Rev. A **42**, 911 (1990); H. Nishimori and T. Nukii, J. Phys. Soc. Jpn. **58**, 563 (1988); S. Puri and C. Roland, Phys. Lett. A **151**, 500 (1990); A. J. Bray and K. Humayun, J. Phys. A **23**, 5897 (1990); T. J. Newman, A. J. Bray, and M. A. Moore, Phys. Rev. B **42**, 4514 (1990).

[3] G. F. Mazenko and M. Zannetti, Phys. Rev. B **32**, 4565 (1985); F. de Pasquale and P. Tartaglia, *ibid.* **33**, 2081 (1986); A. Coniglio and M. Zannetti, Europhys. Lett. **10**, 575 (1989); A. J. Bray, Phys. Rev. B **41**, 6724 (1990); T. J. Newman and A. J. Bray, J. Phys. A **23**, 4491 (1990); A. J. Bray and K. Humayun, Phys. Rev. Lett. **68**, 1559 (1992).

[4] M. Mondello and N. Goldenfeld, Phys. Rev. A **42**, 5865 (1990).

[5] M. Mondello and N. Goldenfeld, Phys. Rev. A **45**, 657 (1992).

[6] I. Chuang, N. Turok, and B. Yurke, Phys. Rev. Lett. **66**, 2472 (1991); I. L. Chuang, R. Durrer, N. Turok, and B. Yurke, Science **251**, 1336 (1991); A. Pargellis, N. Turok, and B. Yurke, Phys. Rev. Lett. **67**, 1570 (1991); A. P. Y. Wong, P. Wiltzius, and B. Yurke, *ibid.* **68**, 3583 (1992).

[7] A. J. Bray and S. Puri, Phys. Rev. Lett. **67**, 2670 (1991); see also H. Toyoki, Phys. Rev. B **45**, 1965 (1992).

[8] Fong Liu and G. F. Mazenko, Phys. Rev. B **45**, 6989 (1992). Note that this paper defines the exponent λ *differently* from the present paper, which uses the notation of Ref. [9]. The sum of the two λ's is d, the spatial dimension.

[9] A. J. Bray and K. Humayun, J. Phys. A **25**, 2191 (1992).

[10] G. Porod, in *Small-Angle X-ray Scattering,* edited by O. Glatter and O. Krattky (Academic, New York, 1982); P. Debye, H. R. Anderson, and H. Brumberger, J. Appl. Phys. **28**, 679 (1957); Y. Oono and S. Puri, Mod. Phys. Lett. B **2**, 861 (1988).

[11] H. Toyoki, J. Phys. Soc. Jpn. **60**, 1153 (1991); **60**, 1433 (1991).

[12] Fong Liu and G. F. Mazenko, Phys. Rev. B **46**, 5963 (1992).

[13] G. F. Mazenko, Phys. Rev. Lett. **63**, 1605; Phys. Rev. B **42**, 4487 (1990).

[14] T. Ohta, D. Jasnow, and K. Kawasaki, Phys. Rev. Lett. **49**, 1223 (1982). This approach was generalized to a two-component vector order parameter by *K.* Kawasaki, Phys. Rev. A **31**, 3880 (1985), with a prediction of $t^{1/2}$ growth for $d=3$; correlation functions, however, were not calculated.

[15] A. J. Bray and K. Humayun (unpublished).

[16] All length scales measured in [5] grow roughly as $t^{0.45}$, rather than $t^{1/2}$ as predicted in Refs. [7–9]. This may indicate that the data are not yet in the asymptotic regime. It should be noted, however, that the $t^{1/2}$ growth law has not been rigorously established for vector systems: Refs. [7–9] all invoke a Gaussian aproximation for the auxiliary field m.

[17] N. Goldenfeld (private communication).

[18] W. H. Zurek, Nature (London) **317**, 505 (1985).