

Velocity distribution of topological defects in phase-ordering systems

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The distribution of interface (domain-wall) velocities \mathbf{v} in a phase-ordering system is considered. Heuristic scaling arguments based on the disappearance of small domains lead to a power-law tail $P_v(v) \sim v^{-p}$, for large v , in the distribution of $v \equiv |\mathbf{v}|$. The exponent p is given by $p = 2 + d/(z-1)$, where d is the space dimension and $1/z$ is the growth exponent, i.e., $z=2$ for nonconserved (model A) dynamics and $z=3$ for the conserved case (model B). The nonconserved result is exemplified by an approximate calculation of the full distribution using a Gaussian closure scheme. The heuristic arguments are readily generalized to systems described by a vector order parameter. [S1063-651X(97)09805-X]

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I. INTRODUCTION

The theory of phase-ordering dynamics has seen significant advances in recent years [1]. Coarsening proceeds by the elimination of topological defects, e.g., domain walls, vortices, or strings, and various properties of the defect distribution have been investigated in some detail [2,3].

In a recent paper, Mazenko [4] has carried out an investigation of the distribution of defect velocities in a phase-ordering system. Using an approximate ‘‘Gaussian closure’’ scheme, he has computed the velocity distribution for point defects in $O(n)$ models with a nonconserved order parameter. He finds the interesting result that the velocity distribution has a power-law tail.

In the present work we shall show that such power-law tails can be deduced rather generally using very simple scaling arguments. The central idea is that large defects velocities are associated with the vanishing of defects at small length scales. Hence the tail gives information about the small-scale structure of the defect morphology. However, the velocity distribution is more cleanly defined and therefore more convenient to study theoretically (and in simulations) than the morphology itself. The physical arguments we shall use are very general and can be applied to systems with both pointlike and extended defects, with or without conservation of the order parameter.

Consider, for example, systems described by a scalar order parameter. This class includes the ‘‘standard’’ phase-ordering systems such as binary alloys (order-disorder transitions or phase separation) and binary liquids. The configuration of the coarsening system is described by the locations of the interfaces, or domain walls, that separate regions occupied by the two ordered phases. We are interested in the velocity distribution of points on the interfaces. The high-velocity tail in the distribution arises as follows. At all stages of the coarsening process, small domains are being eliminated. When the domains are very small, the walls move very quickly. So the high-velocity tail is related to the density of small domains. This is the basic idea behind the scaling argument presented in Sec. II. For the case of nonconserved scalar fields, an explicit calculation using a Gaussian closure scheme (Sec. III) gives an approximate form for the full velocity distribution, extending Mazenko’s work [4]

on the velocity distribution of point defects in $O(n)$ models. The tail of the distribution agrees with the result derived from scaling arguments.

We shall show that an alternative (and *a priori* equally valid) way of using the Gaussian closure results to compute the velocity distribution gives a Gaussian tail rather than a power-law tail. The defect velocity distribution, therefore, is a useful discriminator between various computational schemes. It is reassuring that, in the limit of large spatial dimension d , when the Gaussian closure approximation is believed to become exact (for nonconserved fields), both schemes yield the same results.

In Sec. IV the scaling arguments are extended to vector fields and the general result $p = 2 + (d+1-n)/(z-1)$ is obtained for the tail exponent. For point defects ($n=d$) this result agrees with that obtained by Mazenko [4] using the Gaussian closure approximation. On the basis of the results for scalar fields and vector fields with point defects, we conjecture [Eq. (24)] a general form for the defect velocity distribution within the Gaussian approximation.

II. SCALING APPROACH

A. Nonconserved scalar fields

A system described by a nonconserved scalar field coarsens by curvature driven growth [1]. The normal velocity of a point on an interface is proportional to the total curvature K . For a small circular (or spherical, in $d=3$) domain of radius r , $K = (d-1)/r$. The velocity of the interface is therefore $v = dr/dt \propto -1/r$. It follows that the time t for a domain of initial radius r to disappear scales as $t \propto r^2$.

Let $n(r)dr$ be the number of domains per unit volume with radius between r and $r+dr$. The assumed scaling of the domain morphology gives

$$n(r) = L^{-(d+1)} f(r/L), \quad (1)$$

where $L(t) \sim t^{1/2}$ is the characteristic length scale at time t after the quench into the ordered phase. Integrating Eq. (1) over r gives of order one domain per scale volume L^d , as required by scaling.

In a time interval Δt , domains with $r < (\Delta t)^{1/2}$ will disappear. From Eq. (1) the number of such domains is

$$L^{-(d+1)} \int_0^{(\Delta t)^{1/2}} dr f(r/L) \sim L^{-(d+1)} (dL/dt) \Delta t. \quad (2)$$

The right-hand side of Eq. (2) follows from the fact that the total number of domains per unit volume scales as L^{-d} . The requirement that the left-hand side of Eq. (2) be linear in Δt for $\Delta t \rightarrow 0$ implies the property $f(x) \sim x$, for $x \rightarrow 0$, for the scaling function $f(x)$. Inserting this form into Eq. (2), one recovers $L(t) \sim t^{1/2}$ as expected.

We have shown that $n(r)dr \sim r dr/L^{d+2}$ for $r \ll L$. The interfacial area per unit volume associated with these small domains is

$$A(r)dr \sim r^{d-1} n(r)dr \sim r^d dr/L^{d+2}. \quad (3)$$

Normalizing by the total interfacial area per unit volume L^{-1} gives the area-weighted probability for interfacial radius of curvature between r and $r+dr$, i.e.,

$$P_r(r)dr \sim r^d dr/L^{d+1}, \quad r \ll L. \quad (4)$$

Since the velocity associated with radius of curvature r is $v \sim 1/r$, the interfacial velocity distribution $P_v(v)$ is obtained from $P_v(v) = P_r(r)|dr/dv|$, giving the power-law tail

$$P_v(v) \sim \frac{1}{v(vL)^{d+1}}. \quad (5)$$

This, together with its generalizations below, is our main result.

B. Conserved scalar fields

For conserved scalar fields, coarsening proceeds through the Lifshitz-Slyozov-Wagner (LSW) evaporation-condensation mechanism [5], by which large domains (or, more generally, regions with low interfacial curvature) grow at the expense of small domains (regions of high curvature). This leads to the LSW growth law $L(t) \sim t^{1/3}$. Large domain-wall velocities are associated, as in the nonconserved case, with the disappearance of small domains. For the conserved case, however, the relation between velocity and radius is $v(r) \sim 1/r^2$ [1,5]. Therefore, the time taken for a domain of size $r \ll L(t)$ to evaporate is of order r^3 . In a time interval Δt , domains of size $r < (\Delta t)^{1/3}$ will disappear. Using Eq. (1), the number of such domains is

$$L^{-(d+1)} \int_0^{(\Delta t)^{1/3}} dr f(r/L) \sim L^{-(d+1)} (dL/dt) \Delta t, \quad (6)$$

in complete analogy to Eq. (2). The requirement that the left-hand side be proportional to Δt forces the domain-size distribution function $f(x)$ to have the small- x form $f(x) \sim x^2$ for conserved scalar fields. Inserting this form into Eq. (6), one recovers $L(t) \sim t^{1/3}$ as expected.

The interfacial area per unit volume associated with these small domains is given by $A(r)dr \sim r^{d-1} n(r)dr$, as in Eq. (3). Using $n(r)dr \sim r^2 dr/L^{d+3}$ for $r \ll L$, which follows from $f(x) \sim x^2$, and normalizing by the interfacial area per unit volume L^{-1} gives the area-weighted probability for interfacial radius of curvature between r and $r+dr$:

$$P_r(r)dr \sim r^{d+1} dr/L^{d+2}, \quad r \ll L, \quad (7)$$

instead of Eq. (4). The final step is to use the relation $v \sim 1/r^2$ to deduce the velocity distribution $P_v(v)$ from $P_v(v) = P_r(r)|dr/dv|$. From Eq. (7) one infers the power-law tail

$$P_v(v) \sim \frac{1}{v(vL^2)^{(d+2)/2}} \quad (8)$$

for conserved scalar fields.

The scaling approach adopted for scalar fields can be readily generalized to vector fields. Before doing so, however, we will consider an analytical approach, based on a Gaussian closure scheme, for computing the full distribution $P_v(v)$ (i.e., not just the tail) for the nonconserved scalar case. This is instructive as it provides, in conjunction with the scaling result (5) for the tail, a way of discriminating between two (*a priori* equally valid) ways of using the Gaussian closure results in the calculation of P_v .

III. CALCULATION OF $P_v(v)$ USING GAUSSIAN CLOSURE

The idea underlying all Gaussian closure schemes is the introduction of a ‘‘smooth’’ auxiliary field $m(\mathbf{x}, t)$ whose zeros define the interfaces, i.e., m has its zeros at the same points as the order-parameter field $\phi(\mathbf{x}, t)$. Whereas ϕ is essentially constant within domains, but varies rapidly within domain walls, m is smooth, i.e., it varies only on the larger scale $L(t)$. At this stage, however, it is not necessary to specify precisely how m is defined.

An expression for the interface velocity in terms of m can be obtained by noting that the rate of change of m in a frame moving with the interface is zero, i.e., $dm/dt = 0 = \partial m / \partial t + \mathbf{v} \cdot \nabla m$. Since ∇m is normal to the interface, $\mathbf{v} \cdot \nabla m = v_n |\nabla m|$, where v_n is the normal velocity of the interface. This gives

$$v_n(\mathbf{x}) = -\partial_t m / |\nabla m|. \quad (9)$$

Formally this equation defines a ‘‘velocity’’ at every point: the velocity of the surface of constant m defined at that point. To find the distribution of interface velocities, we have to project onto the interfaces:

$$P_v(v) = \frac{\langle \delta(v - v_n(\mathbf{x})) \rho(\mathbf{x}) \rangle}{\langle \rho(\mathbf{x}) \rangle}, \quad (10)$$

where $\rho(\mathbf{x})$ is the areal density of interface, given by

$$\rho(\mathbf{x}) = \delta(m(\mathbf{x})) |\nabla m|. \quad (11)$$

Integrating $\rho(\mathbf{x})$ over any volume of space gives the interfacial area in that volume.

Equations (9)–(11) are exact, but in order to make further progress one needs to know the joint distribution function for m , $\partial_t m$, and the components $\partial_i m$ of ∇m , at a given point in space. In all Gaussian closure schemes, the field $m(\mathbf{x}, t)$ is assumed to be Gaussian. This approximation works reasonably well in practice for nonconserved fields [1]. Using it, the required distribution function is expressible in terms of

the inverse of the covariance matrix of the variables m , $\dot{m} \equiv \partial_t m$, and $\partial_i m$ ($i=1, \dots, d$). Clearly $\langle m \partial_i m \rangle$ and $\langle \dot{m} \partial_i m \rangle$ both vanish due to translational invariance. Similarly, $\langle \partial_i m \partial_j m \rangle$ vanishes for $i \neq j$ due to the assumed isotropy of the system. It follows that the only nonzero elements of the covariance matrix are $S(t) = \langle m^2 \rangle$, $\dot{S}/2 = \langle m \dot{m} \rangle$, $T(t) = \langle \dot{m}^2 \rangle$, and $U(t) = \langle (\partial_i m)^2 \rangle$. Note that the ∇m sector is decoupled from the (m, \dot{m}) sector. The required probability distribution has, therefore, the product form

$$P(m, \dot{m}, \nabla m) = \frac{1}{(2\pi U)^{d/2}} \exp\left(-\frac{(\nabla m)^2}{2U}\right) \frac{1}{2\pi D} \times \exp\left(-\frac{1}{2D}(Tm^2 - \dot{S}m\dot{m} + S\dot{m}^2)\right), \quad (12)$$

where

$$D = ST - \dot{S}^2/4 \quad (13)$$

is the determinant of the covariance submatrix in the (m, \dot{m}) sector.

From Eqs. (10) and (11) the velocity distribution is given by

$$P_v(v) = \frac{\langle \delta(v + \dot{m}/|\nabla m|) \delta(m) |\nabla(m)| \rangle}{\langle \delta(m) |\nabla(m)| \rangle}. \quad (14)$$

Evaluating the averages using the distribution (12) gives

$$P_v(v) = \frac{1}{\sqrt{\pi}} \frac{\Gamma\left(\frac{d+2}{2}\right)}{\Gamma\left(\frac{d+1}{2}\right)} \frac{1}{\bar{v}} \frac{1}{(1+v^2/\bar{v}^2)^{(d+2)/2}}, \quad (15)$$

where the characteristic velocity \bar{v} is given by

$$\bar{v} = \sqrt{\frac{D}{SU}} = \sqrt{\frac{\langle m^2 \rangle \langle \dot{m}^2 \rangle - \langle m \dot{m} \rangle^2}{\langle m^2 \rangle \langle (\nabla m)^2 \rangle / d}}. \quad (16)$$

Note that the distribution (15) is normalized on the interval $(-\infty, \infty)$.

The $v^{-(d+2)}$ tail predicted by Eq. (15) agrees with the scaling arguments for nonconserved fields presented in Sec. II. This agreement is a nontrivial result, since up to now we have made no assumptions about the nature of the dynamics. The only assumption used is that the field m is Gaussian, which is evidently qualitatively correct for nonconserved fields but not for conserved fields, where the power law predicted using Eq. (15) disagrees with the scaling result (8). We conclude that no simple Gaussian auxiliary-field approach captures the physics of the conserved model. Similar conclusions have been drawn in another context [9].

The explicit value of \bar{v} in Eq. (16) depends on the dynamics of the field m . The simplest approximation is that of Ohta, Jasnow, and Kawasaki [6], in which m obeys the diffusion equation $\partial_t m = D_0 \nabla^2 m$, with $D_0 = (d-1)/d$. The initial condition is $\langle m(\mathbf{x}, 0) m(\mathbf{x}', 0) \rangle = \Delta \delta(\mathbf{x} - \mathbf{x}')$. With this

choice one obtains $\bar{v} = [(d-1)/2t]^{1/2}$. Other approximations, such as that of Mazenko [7], give the same $t^{-1/2}$ behavior, but with a different prefactor. The $t^{-1/2}$ dependence follows quite generally from the scaling relation $\bar{v} \sim dL/dt$ and the usual result $L \sim t^{1/2}$ for nonconserved scalar fields.

Before concluding this section, it is instructive to briefly discuss an alternative approach [8] to implementing the Gaussian assumption for the field m . Consider a given mapping $\phi(m)$ between the original field ϕ and the auxiliary field m . The spatial variation of ϕ across an interface is asymptotically identical (in the scaling regime) to that of an equilibrium interface. It follows that, at an interface, $|\nabla \phi|$ is a given constant, determined by the equilibrium interface profile, and therefore $|\nabla m|$ is a constant, which we shall call a .

This discussion shows that the Gaussian approximation cannot be exact because, for a Gaussian field m , $|\nabla m|$ fluctuates with position on the interface. An exception is the limit $d \rightarrow \infty$, when $|\nabla m|$ approaches the limit $[\sum_{i=1}^d \langle (\partial m / \partial x_i)^2 \rangle]^{1/2}$. We shall return to this limit below.

Replacing $|\nabla m|$ by a in Eqs. (9) and (11) leads to the probability distribution

$$P_v(v) = \frac{\langle \delta(v + \dot{m}/a) \delta(m) \rangle}{\langle \delta(m) \rangle} = \left(\frac{Sa^2}{2\pi D}\right)^{1/2} \exp\left(-\frac{Sa^2}{2D}v^2\right). \quad (17)$$

This new approach, therefore, fails to reproduce the power-law tail in $P_v(v)$ predicted using the general arguments presented in Sec. II, but gives instead a Gaussian distribution for all d . While both approaches would seem to be equally valid *a priori*, the calculation of $P_v(v)$ discriminates clearly in favor of the first approach of treating the field m consistently as Gaussian throughout. In the limit $d \rightarrow \infty$, however, both approaches agree, since Eq. (15) has, for large d , the limiting Gaussian form

$$P_v(v) = (t/\pi)^{1/2} \exp(-tv^2), \quad (18)$$

using $\bar{v} \rightarrow (d/2t)^{1/2}$ from the Ohta-Jasnow-Kawasaki (OJK) theory.

A concrete realization of the new scheme requires a model that ensures that the interface thickness is time independent. Although it is difficult to enforce the constraint $|\nabla m| = a$ at interfaces, models in which the looser condition $\langle (\nabla m)^2 \rangle = a^2$ is imposed can be devised. The simplest such model is that proposed by Bray and Humayun [1,10], which is equivalent to the Oono-Puri extension [11] of the OJK model. Within this model, the field is still strictly Gaussian, so $P_v(v)$ still has the form (15). This model allows, however, a quantitative comparison of Eqs. (17) and (15) for $d \rightarrow \infty$. One finds [1,10] $S = 4t/d$, $T = (d+2)/2dt$, and $U = 1/d$ (corresponding to $a = 1$), and hence $D = 2/d$. Putting these results into either Eq. (15), with $d \rightarrow \infty$, or Eq. (17), with $a = 1$, reproduces Eq. (18).

IV. VECTOR FIELDS

The scaling arguments of Sec. II can be generalized rather simply to n -component vector fields in spatial dimension $d \geq n$ (the latter condition being necessary for the existence

of localized defects). The quantitative (though approximate) methods of Sec. III are, for technical reasons, less straightforward to extend to the general case. Mazenko [4] has recently given the result for nonconserved fields with point defects ($n=d$).

The scaling argument can be presented in a rather general way. If the dynamical exponent is z , i.e., $L(t) \sim t^{1/z}$, it follows that the characteristic velocity scales as $dL/dt \sim L^{-(z-1)}$. The next step is to assume that a small defect structure [a small domain ($n=1$), a small vortex loop ($n=2, d=3$), or vortex-antivortex pair ($n=2=d$), etc.], of size much less than $L(t)$, collapses under its own internal forces at a rate consistent with scaling. That is, the scale r of the structure evolves as $dr/dt \sim -r^{-(z-1)}$ for $r \ll L(t)$. The collapse time of such a structure will then scale as r^z and structures with $r < (\Delta t)^{1/z}$ will disappear in a time interval Δt . This scenario agrees precisely with what we found explicitly for scalar fields in Sec. II, where $z=2$ (3) for nonconserved (conserved) fields. The case $n=2$ has been discussed by Rutenberg and Bray [12].

The number of defect structures per unit volume with size between r and $r+dr$ is again given by the scaling form (1). Requiring that the number of structures that disappear in interval Δt be linear in Δt forces the scaling function $f(x)$ in Eq. (1) to have the small-argument form $f(x) \sim x^{z-1}$, giving $n(r) \sim r^{z-1}/L^{d+z}$ for $r \ll L$. The core volume of a structure of size r scales as r^{d-n} , while the total core volume per unit volume of space scales as L^{-n} . The core-volume weighted probability for defect structure size between r and $r+dr$ is, therefore,

$$P_r(r)dr \sim r^{z-1+d-n}dr/L^{d+z-n}, \quad r \ll L, \quad (19)$$

a generalization of Eqs. (4) and (7). Using $v \sim r^{-(z-1)}$ leads to the power-law tail

$$P_v(v) \sim \frac{1}{v(vL^{z-1})^{p-1}}, \quad (20)$$

with the tail-exponent

$$p=2+(d+1-n)/(z-1). \quad (21)$$

This result generalizes Eqs. (5) and (8), to which it reduces for $n=1$ and $z=2,3$, respectively.

We can compare this result with the analytical result for $P_v(v)$ obtained using the Gaussian closure approximation for nonconserved fields ($z=2$) with point defects ($n=d$) [4]. For this case Eq. (21) becomes $p=3$, i.e., $P_v(v) \sim 1/L^2v^3$. Note that $P_v(v)$ is the probability distribution for the *magnitude* of the velocity. The Gaussian closure calculation gives an expression for the probability distribution $P(\vec{v})$ of the *vector* velocity in the form [4]

$$P(\vec{v}) = \frac{\Gamma\left(\frac{n+2}{2}\right)}{(\pi\bar{v}^2)^{n/2}} \frac{1}{(1+v^2/\bar{v}^2)^{(n+2)/2}}. \quad (22)$$

The normalization of this distribution is $\int d^n v P(\vec{v}) = 1$, whereas $P_v(v)$ is normalized as $\int_0^\infty dv P_v(v) = 1$. The rela-

tion between these two distributions is simply $P_v(v) = [2\pi^{n/2}/\Gamma(n/2)]v^{n-1}P(v)$, i.e.,

$$P_v(v) = \frac{n}{\bar{v}} \frac{(v/\bar{v})^{n-1}}{(1+v^2/\bar{v}^2)^{(n+2)/2}}. \quad (23)$$

The power-law tail is $P_v(v) \sim n\bar{v}^2/v^3$, which agrees with the scaling result (21) (for the case $n=d, z=2$).

V. CONCLUSION

The velocity distribution of topological defects in a phase-ordering system has been discussed. A simple scaling argument, introduced in the context of domain walls in Sec. II and generalized to vector fields in Sec. IV, predicts a power-law tail at large velocity. The tail exponent p is given by the general result (21), where z is the dynamical exponent that describes the coarsening dynamics, via $L(t) \sim t^{1/z}$.

For the special case of nonconserved fields, approximate analytical calculations, based on a Gaussian closure scheme, have been performed for scalar fields (Sec. III) and for vector fields with point defects [4]. In both cases the approximate result exhibits the power-law tail predicted by the scaling arguments. A comparison of Eqs. (15) and (23) suggests the following conjecture for general nonconserved vector fields, within the Gaussian approximation:

$$P_v(v) = \frac{2\Gamma\left(\frac{d+2}{2}\right)}{\Gamma\left(\frac{n}{2}\right)\Gamma\left(\frac{d-n+2}{2}\right)} \frac{1}{\bar{v}} \frac{(v/\bar{v})^{n-1}}{(1+v^2/\bar{v}^2)^{(d+2)/2}}. \quad (24)$$

This result reduces to Eq. (15) for $n=1$ [13], to Eq. (23) for $n=d$, and gives rise to the power-law tail $P_v(v) \sim v^{-p}$ with $p=d+3-n$, in agreement with the scaling prediction (21) for $z=2$.

As a final comment we note that for certain systems the growth law for $L(t)$ is expected to contain logarithmic corrections to a simple power law. Two examples are the nonconserved $n=2$ model for $d=2$, where one expects [12,14] $L(t) \sim (t/\ln t)^{1/2}$, and the conserved $n=2$ model for $d \geq 3$, where [12,15] $L(t) \sim (t/\ln t)^{1/4}$. A simple scaling approach of the type used in Secs. II and IV cannot be applied naively, due to the appearance of a new length scale, the defect core size, which enters as a short-scale cutoff in the logarithms. We would expect, however, that any resulting modifications of the final result would be limited to possible logarithmic corrections to the power-law tail in $P_v(v)$. The dominant power-law part will be obtained by inserting the appropriate value of z (2 or 4, respectively, in the cases discussed above) in Eq. (21).

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