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Towards a systematic calculation of the scaling functions for the ordering kinetics of nonconserved fields

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A systematic approach to the solution of the time-dependent Ginzburg-Landau equation for a nonconserved field, with random initial conditions appropriate to a quench from the disordered to the ordered phase, is introduced. In leading order, the scaling functions for two-point correlations have the Ohta-Jasnow-Kawasaki form and its generalization to vector fields.

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The field of phase-ordering kinetics — the evolution of large-scale structure, with scale-invariant morphology, following the rapid quench of a system from its disordered to ordered phases — continues to fascinate theorist and experimentalist alike [1]. Although the growth laws that describe the asymptotic time dependence of the structure are, at least for scalar fields, well understood [2] and there is a well-developed scaling phenomenology for describing the late stages of growth [3], the first-principles calculation of correlation functions remains a challenge to the theorist. A number of approximate theories have been advanced [4–9], but a systematic approach has proved elusive. Indeed, the very existence of scaling has been questioned for systems with a *conserved* order parameter [10].

Exact results, or soluble limits, in the theory of ordering kinetics are few in number [11]. In this Rapid Communication we present, for the first time, a systematic approach to the solution of the time-dependent Ginzburg-Landau (TDGL) equation for a nonconserved field, with random initial conditions. In leading order our approach reproduces, for a scalar field, the well-known scaling function of Ohta, Jasnow, and Kawasaki (OJK) [5]. For a vector field it gives the generalization of the OJK function recently derived by Bray and Puri, and by Toyoki (BPT) [7].

For simplicity of presentation, we will begin with scalar fields. The extension to vector fields is relatively simple and will be sketched at the end. The TDGL equation for a nonconserved scalar field $\phi(\mathbf{x},t)$ reads

$$\partial_t\phi=\nabla^2\phi-V'(\phi)\ , \tag{1}$$

where $V(\phi)$ is a symmetric double-well potential, with minima at $\phi=\pm1$, and $V'(\phi)\equiv\partial V/\partial\phi$. The detailed form of $V(\phi)$, however, should not be important, a fact that we will exploit.

The absence of a thermal noise term in (1) indicates that we are working at temperature $T=0$. There are good reasons to believe that temperature is an irrelevant variable (for $T<T_C$), since phase ordering should be controlled (assuming the scaling hypothesis [3] is valid) by a "strong-coupling" (or $T=0$) renormalization-group fixed point [12]. In practice this means that universal scaling is expected when the "domain scale" $L(t)$ is large compared to the thermal correlation length ξ of the equilibrium ordered phase. At $T=0$, the scaling regime occurs when $L(t)$ is large compared to the intrinsic width w of domain walls, obtained from the equilibrium solution of (1) for a single wall.

Equation (1) has to be supplemented by a distribution function for the random initial conditions that specify the state immediately after the quench. Then the quantity of principal interest is the two-point correlation function

$$C(\mathbf{r},t)=\langle\phi(\mathbf{x},t)\phi(\mathbf{x}+\mathbf{r},t)\rangle\ , \tag{2}$$

where angle brackets indicate an average over initial conditions. If the scaling hypothesis holds, then

$$C(\mathbf{r},t)=f(r/L(t))\ , \tag{3}$$

where, as discussed above, $L(t)$ is a time-dependent characteristic scale (domain scale). The calculation of $C(r,t)$ from first principles, starting from (1), is highly nontrivial.

A significant simplification may be achieved by introducing a new field $m(\mathbf{x},t)$, following the approach of Mazenko [6] in his approximate calculation of $C(\mathbf{r},t)$. Specifically, we define the function $\phi(m)$ by the equation

$$\phi''(m)=V'(\phi)\ , \tag{4}$$

where primes indicate derivatives, with boundary conditions $\phi(\pm\infty)=\pm1$. Comparing (4) with (1) we see that $\phi(m)$ is just the equilibrium domain-wall profile function, with m playing the role of the distance from the wall. The additional condition $\phi(0)=0$ locates the center of the wall at $m=0$. Rewriting (1) in terms of m, and using (4) to eliminate V', gives

$$\partial_t m=\nabla^2 m-\frac{\phi''(m)}{\phi'(m)}[1-(\nabla m)^2]\ . \tag{5}$$

For general potentials $V(\phi)$, Eq. (5) is a complicated nonlinear equation, not obviously simpler than the original TDGL equation (1). It is, however, widely believed that the scaling function $f(x)$ is *independent* both of the detailed form of the potential and of the particular choice for the distribution of initial conditions. The reason is as follows. Physically, the motion of the interfaces (or domain walls) is driven by their *curvature*. The potential

$V(\phi)$ determines the domain-wall *profile,* which is irrelevant to the large-scale structure. The Allen-Cahn theory [13], derived from Eq. (1), gives an explicit expression for the domain-wall velocity in terms of the local curvature, $v_n = -\nabla\cdot\mathbf{n}$, where $\mathbf{n}$ is the normal to the wall (in the direction, say, of increasing ϕ), and v_n is the velocity of the wall along $\mathbf{n}$. For example, for a single spherical domain of one phase, in a sea of the other phase, the Allen-Cahn equation gives $\partial_t R = -(d-1)/R$ for the radius R of the domain, independent of the details of the potential. This equation for R can be verified directly from (1) for R large compared to the width w of the wall.

Similarly, the initial conditions determine the early-time locations of the walls, which should again be irrelevant for late-stage scaling properties. For example, in Mazenko's approximate theory [6], both the potential and the initial conditions drop out from the equation for $f(x)$.

The key step in our approach is to exploit the notion that the scaling function should be independent of the potential (or, equivalently, independent of the wall profile) by choosing a particular $V(\phi)$ such that Eq. (5) takes a much simpler form [Eq. (9)]. Specifically we choose the domain-wall profile function $\phi(m)$ to satisfy

$$\phi''(m) = -m\phi'(m) \ . \tag{6}$$

This is equivalent, via (4), to a particular choice of potential, as discussed below. First we observe that (6) can be integrated, with boundary conditions $\phi(\pm\infty)=\pm 1$ and $\phi(0)=0$ to give the wall profile function

$$\phi(m) = (2/\pi)^{1/2}\int_0^m dx\, \exp(-x^2/2)$$
$$= \mathrm{erf}(m/\sqrt{2}) \ , \tag{7}$$

where $\mathrm{erf}(x)$ is the error function. Also, (4) can be integrated once, with the zero of potential defined by $V(\pm 1)=0$, to give

$$V(\phi) = \tfrac{1}{2}(\phi')^2 = (1/\pi)\exp(-m^2)$$
$$= (1/\pi)\exp\{-2[\mathrm{erf}^{-1}(\phi)]^2\} \ , \tag{8}$$

where $\mathrm{erf}^{-1}(x)$ is the inverse function of $\mathrm{erf}(x)$. In particular, $V(\phi)\simeq 1/\pi - \phi^2/2$ for $\phi^2 \ll 1$, while $V(\phi)\simeq \frac{1}{4}(1-\phi^2)^2|\ln(1-\phi^2)|$ for $(1-\phi^2)\ll 1$ [14]. With the choice (6), Eq. (5) reduces to the much simpler equation

$$\partial_t m = \nabla^2 m + [1-(\nabla m)^2]m \ . \tag{9}$$

This equation, though still nonlinear, represents a significant simplification of the original TDGL equation. We believe, however, on the basis of the physical arguments discussed above, that it retains all the ingredients necessary to describe the universal scaling properties [15]. Equation (9) should therefore serve as a useful starting point for future studies.

We now proceed to show that the usual OJK and BPT results are recovered by simply replacing $(\nabla m)^2$ by its average (over the ensemble of initial conditions) in (9), and choosing a Gaussian distribution for the initial conditions. In order to make this replacement in a controlled way, however, and to facilitate the computation of corrections to the leading-order results, we systematize the treatment by attaching to the field m an internal "color" index α, which runs from 1 to N, and generalize (9) to

$$\partial_t m_\alpha = \nabla^2 m_\alpha + \left[1 - N^{-1}\sum_{\beta=1}^{N}(\nabla m_\beta)^2\right]m_\alpha \ .$$

Equation (9) is the case $N=1$. The OJK and BPT results are obtained, however, by taking the limit $N\to\infty$, when $N^{-1}\sum_{\beta=1}^{N}(\nabla m_\beta)^2$ may be replaced by its average. With this simplification (9) becomes (where m now stands for one of the m_α)

$$\partial_t m = \nabla^2 m + a(t)m \ , \tag{10}$$

$$a(t) = 1 - \langle(\nabla m)^2\rangle \ , \tag{11}$$

a self-consistent *linear* equation for $m(\mathbf{x},t)$.

It is interesting that the replacement of $(\nabla m)^2$ by its average in (9) is also justified in the limit $d\to\infty$, where d is the number of spatial dimensions, because $(\nabla m)^2 = \sum_{i=1}^{d}(\partial m/\partial x_i)^2$. If m is a Gaussian random field [and the self-consistency of this assumption follows from (10) — see below], then the different derivatives $\partial m/\partial x_i$ at a given point x are independent random variables, and the central limit theorem gives, for $d\to\infty$, $(\nabla m)^2 \to d\langle(\partial m/\partial x_i)^2\rangle = \langle(\nabla m)^2\rangle$, with fluctuations of relative order $1/\sqrt{d}$. While this approach is not so simple to systematize as that adopted above it seems very likely that our leading-order results become exact for large d.

As discussed above, we will take the initial conditions for m to be Gaussian, with mean zero and correlator (in Fourier space)

$$\langle m_{\mathbf{k}}(0)m_{-\mathbf{k}'}(0)\rangle = \Delta\delta_{\mathbf{k},\mathbf{k}'} \ , \tag{12}$$

representing short-range spatial correlations at $t=0$. Then m is a Gaussian field at all times. The solution of (10) is $m_{\mathbf{k}}(t) = m_{\mathbf{k}}(0)\exp[-k^2 t + b(t)]$, where $b(t) = \int_0^t dt' a(t')$. Inserting this into (11) yields

$$a(t) \equiv \frac{db}{dt} = 1 - \Delta\sum_{\mathbf{k}} k^2 \exp(-2k^2 t + 2b) \ .$$

After evaluating the sum, one obtains, for large t (where the db/dt term can be neglected), $\exp(2b)\simeq(4t/\Delta d)(8\pi t)^{d/2}$, and hence $a(t)\simeq(d+2)/4t$. This form for $a(t)$ in (10), arising completely naturally in this scheme, reproduces exactly the "Oono-Puri extension" to the OJK theory, an *ad hoc* addition to OJK's diffusion equation for m, designed to keep the wall width fixed as $t\to\infty$ [16].

The explicit result for $m_k(t)$, valid for large t, is

$$m_k(t) = m_k(0)(4t/\Delta d)^{1/2}(8\pi t)^{d/4}\exp(-k^2 t) \ , \tag{13}$$

from which the equal-time two-point correlation functions in Fourier and real space follow immediately:

$$\langle m_k(t)m_{-k}(t)\rangle = (4t/d)(8\pi t)^{d/2}\exp(-2k^2 t) \ , \tag{14}$$

$$\langle m(1)m(2)\rangle = (4t/d)\exp(-r^2/8t) \ , \tag{15}$$

where 1,2 are a shorthand for space-time points $(\mathbf{r}_1,t)$, $(\mathbf{r}_2,t)$, and $r=|\mathbf{r}_1-\mathbf{r}_2|$.

We turn now to the evaluation of the correlation function (2) of the original fields ϕ. Since, from (15), m is typically of order $\sqrt{t}$ at late times, it follows from (7) that the field ϕ is saturated (i.e., $\phi=\pm1$) almost everywhere at late times. As a consequence, the relation (7) between ϕ and m may be simplified to $\phi=\mathrm{sgn}(m)$ as far as the late time scaling behavior is concerned. Thus $C(12)=\langle \mathrm{sgn}[m(1)]\mathrm{sgn}[m(2)]\rangle$. The calculation of this average for a Gaussian field m is by now standard (see, for example, [16]). The result is

$$C(12)=(2/\pi)\sin^{-1}[\gamma(12)]\ , \tag{16}$$

$$\gamma(12)=\frac{\langle m(1)m(2)\rangle}{\sqrt{\langle m(1)^2\rangle\langle m(2)^2\rangle}}=\exp(-r^2/8t)\ . \tag{17}$$

This result, which has the scaling form (3) with $L(t)\propto\sqrt{t}$, is identical to that derived by OJK by considering the motion of the domain walls [5]. The present approach, however, makes possible a systematic treatment in powers of $1/N$. The work involved in calculating the next term is comparable to that required to obtain the $O(1/n)$ correction to the $n=\infty$ result for the O(n) model [17]. Note, however, that our approach is very different in spirit from the conventional $1/n$ expansion: sharp domain walls, whose existence is essential to a correct description of the underlying physics, are built in through the nonlinear mapping (4).

For vector fields, the TDGL equation reads $\partial\boldsymbol{\phi}/\partial t=\nabla^2\boldsymbol{\phi}-\partial V/\partial\boldsymbol{\phi}$, where $V(\boldsymbol{\phi})$ is the usual "Mexican hat" potential with ground-state manifold $\boldsymbol{\phi}^2=1$. This time we introduce a *vector* field $\mathbf{m}(x,t)$, related to $\boldsymbol{\phi}$ by the vector analog of (4), namely [8,9]

$$\nabla_m^2\boldsymbol{\phi}=\frac{\partial V}{\partial\boldsymbol{\phi}}\ , \tag{18}$$

where ∇_m^2 means $\sum_{a=1}^{n}\partial^2/\partial m_a^2$ for an n-component field. We look for a radially symmetric solution of (18), $\boldsymbol{\phi}(\mathbf{m})=\hat{\mathbf{m}}g(\rho)$, with boundary conditions $g(0)=0$, $g(\infty)=1$, where $\rho=|\mathbf{m}|$ and $\hat{\mathbf{m}}=\mathbf{m}/\rho$. Then the function $g(\rho)$ is the defect profile function for a topological defect in the n-component field, with ρ representing the distance from the defect core. In terms of $\mathbf{m}$, the TDGL equation for a vector field reads

$$\sum_b\frac{\partial\phi_a}{\partial m_b}\frac{\partial m_b}{\partial t}=\sum_b\frac{\partial\phi_a}{\partial m_b}\nabla^2 m_b+\sum_{b,c}\frac{\partial^2\phi_a}{\partial m_b\partial m_c}\nabla m_b\cdot\nabla m_c-\nabla_m^2\phi_a\ . \tag{19}$$

Just as in the scalar theory, we can attach an additional "color" index α $(=1,\ldots,N)$ to the vector field $\mathbf{m}$, such that the theory in the limit $N\to\infty$ is equivalent to replacing $\nabla m_b\cdot\nabla m_c$ by its mean, $\langle(\nabla m_b)^2\rangle\delta_{bc}$ in (19). Noting also that $\langle(\nabla m_b)^2\rangle$ is independent of b from global isotropy, (19) simplifies to

$$\sum_b\frac{\partial\phi_a}{\partial m_b}\frac{\partial m_b}{\partial t}=\sum_b\frac{\partial\phi_a}{\partial m_b}\nabla^2 m_b-\nabla_m^2\phi_a[1-\langle(\nabla m_1)^2\rangle]\ , \tag{20}$$

where m_1 is any component of $\mathbf{m}$. Finally, this equation can be reduced to the linear form (10), with m replaced by $\mathbf{m}$, through the choice $\nabla_m^2\phi_a=-\sum_b(\partial\phi_a/\partial m_b)m_b$ or, more compactly, $\nabla_m^2\boldsymbol{\phi}=-(\mathbf{m}\cdot\nabla_m)\boldsymbol{\phi}$, to determine the function $\boldsymbol{\phi}(\mathbf{m})$. Substituting the radially symmetric form $\boldsymbol{\phi}=\hat{\mathbf{m}}g(\rho)$ gives the equation

$$g''+\left[\frac{n-1}{\rho}+\rho\right]g'-\frac{n-1}{\rho^2}g=0\ , \tag{21}$$

a generalization of (6), for the profile function $g(\rho)$, with boundary conditions $g(0)=0$, $g(\infty)=1$. The solution is linear in ρ for $\rho\to0$, while $g(\rho)\simeq1-(n-1)/2\rho^2$ for $\rho\to\infty$. The potential $V(\boldsymbol{\phi})$ corresponding to this profile function can be deduced from (18), though we have been unable to derive a closed-form expression for it. Note that we are making here the natural assumption that scaling functions are independent of the details of the potential for vector fields, as well as for scalar fields.

For the vector theory, Eqs. (10) and (11) hold separately for each component of the field. Taking Gaussian initial conditions, with correlator (12), yields $a(t)\simeq(d+2)/4t$ again, giving (15) for each component. The final step is the evaluation of the two-point function $C(12)=\langle\boldsymbol{\phi}(1)\cdot\boldsymbol{\phi}(2)\rangle$, analogous to (2). Since $|\mathbf{m}|$ scales as $\sqrt{t}$, we can replace the function $\boldsymbol{\phi}(\mathbf{m})$ by $\hat{\mathbf{m}}$ at late times. Then $C(12)=\langle\hat{\mathbf{m}}(1)\cdot\hat{\mathbf{m}}(2)\rangle$ in the scaling regime. The required Gaussian average over the fields $\mathbf{m}(1)$, $\mathbf{m}(2)$ yields finally [7–9]

$$C(12)=\frac{n\gamma}{2\pi}\left[B\left(\frac{n+1}{2},\frac{1}{2}\right)\right]^2F\left(\frac{1}{2},\frac{1}{2};\frac{n+2}{2};\gamma^2\right)\ , \tag{22}$$

where $B(x,y)$ is the beta function, $F(a,b;c;z)$ the hypergeometric function, and $\gamma\equiv\gamma(12)$ is given once more by (17).

The result (22) is identical to that derived by BPT [7] using an approximate treatment of the TDGL equation, based on the method of Kawasaki, Yalabik, and Gunton [4]. The present paper shows that the BPT result becomes exact for large N, verifying both the existence of scaling and the $\sqrt{t}$ growth law in this limit. The most interesting feature of (22) is a short-distance singularity of the form x^n (or $x^n\ln x$ for n an even integer), where $x=r/\sqrt{t}$ is the scaling variable, leading to a power-law tail in the structure factor [the Fourier transform of $C(12)$], $S(k,t)\sim t^{-n/2}k^{-(d+n)}$ for $k\sqrt{t}\gg1$, and generalizing the familiar "Porod's law" [18] to vector systems. There has been recent interest in looking for these tails in liquid-crystal systems [19]. Subsequent work [20,21] has shown that such tails are a simple consequence of the existence of topologically stable defects, and should therefore be present only for $n\le d$. Furthermore, the *amplitude* of the tail is fixed by purely geometrical considerations, and can be calculated exactly, for

any $n \leq d$, in terms of the defect density [21]. The result agrees with that obtained from (22) for d large at fixed n. That (22), naively applied, yields power-law tails for *any* n and d is another indication that (22) may really be a large-d result. Despite this, however, it fits simulation data for $d=2,3$, with $n \leq d$, rather well [22].

We conclude with a simple extension of the present calculation: "Different-time" correlation functions can be readily computed from the general result (13). The same forms (16) and (22) are obtained, but with

$$\gamma(12)=\left[\frac{4t_1t_2}{(t_1+t_2)^2}\right]^{d/4}\exp\left[-\frac{r^2}{4(t_1+t_2)}\right],$$

which reduces to (17) for $t_1=t_2=t$. This form for γ is the same as that obtained by Yeung and Jasnow [23] from the OJK approach. For $t_2 \gg t_1, C(12) \rightarrow (4t_1/t_2)^{d/4}\exp(-r^2/4t_2)$ (for any n), from which one identifies the "two-time" exponent λ [defined by $C(12)=(L_1/L_2)^{d-\lambda}h(r/L_2)$ for $L_2 \gg L_1$, where $L_1 \equiv L(t_1)$, etc. [24]] as $\lambda=d/2$.

In summary, a systematic approach to the calculation of correlation functions in phase-ordering kinetics has been introduced. At leading order we recover, in a controlled way, the results previously derived as approximations by OJK and BPT for nonconserved scalar and vector fields, respectively. The scaling hypothesis is confirmed for nonconserved fields, and a $\sqrt{t}$ growth law obtained explicitly for both scalar and vector fields. Our approach, based on judicious choices for the potential function and the distribution of initial conditions, opens the door to systematic calculations in powers of $1/N$ (with N the number of "colors" in an extended theory), an avenue we are currently exploring. The intriguing possibility that a similar approach can be usefully exploited for conserved fields is also under consideration.

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