ARTICLES

Ordering kinetics of defect structures

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We show how the continuity equations expressing conservation of topological point or string defect charge can be used to determine the order-parameter correlation function for the phase-ordering kinetics of the $O(n)$ model in the special case where the order parameter is constrained to be near a defect core. In this regime we find a self-consistent solution by assuming the order parameter is Gaussian. The resulting linear equation for the order-parameter correlation function has as its solution the Ohta-Jasnow-Kawasaki form. [S1063-651X(98)04903-4]

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We show here that the phase-ordering kinetics of defects in the $O(n)$ model can be self-consistently evaluated assuming that, infinitesimally close to the defect cores, the order parameter is a Gaussian field. This, in turn, clarifies the nature of recent determinations of defect correlation functions for the $O(n)$ model [1–3]. We consider systems with either point defects ($n=d$, where d is the spatial dimensionality) or string defects ($n=d-1$). In addition to their importance in condensed matter, these systems are also relevant to problems in cosmological structure formation [4]. Our approach is based on the recently derived [5] continuity equation expressing conservation of topological defect charge and differs from previous calculations that make more direct use of the time-dependent Ginzburg-Landau (TDGL) equation for the nonconserved order parameter [6,7]. The continuity equation for systems supporting string defects has not appeared previously and is established here. These continuity equations are used to find the equation satisfied by the order-parameter correlation function where the order parameter is restricted to be infinitesimally close to a defect core. Since it is easy to confuse the usual order-parameter correlation function with the correlation function for the order parameter constrained to be near a defect core, we will, for reasons that will become clear below, refer to this constrained quantity as the auxiliary field correlation function f. We obtain a linear equation for f that has as its solution the Ohta-Jasnow-Kawasaki (OJK) [8] form. Since the equation is linear, the Gaussian assumption is consistent.

Most of the focus in phase-ordering kinetics has been on developing theories for the order-parameter correlation function. The belief has developed that we have a fairly good understanding of how to calculate this quantity in the late-time scaling regime. Two theories have evolved that map the order-parameter field onto an auxiliary field and invoke the so-called Gaussian closure approximation. Since these theories determine the auxiliary field correlation function using a method that is seemingly independent from the one used here, we shall refer to the correlation function for this unconstrained auxiliary field as $f_{\rm OP}$. The OJK method, with elaborations by others [9,10], leads to a simple form for the auxiliary field correlation function. The second approach, originated by Mazenko [6], determines $f_{\rm OP}$ self-consistently through the solution of a nonlinear eigenvalue problem. A key point we make here is that it is not necessary that $f=f_{\rm OP}$.

Since the order-parameter correlation function is a rather structureless quantity that does not give a great deal of direct information about the underlying disordering agents, Liu and Mazenko [1] examined the correlations between the defects themselves. The key element in this work was, following Halperin [11], to identify the positions of the defects with the zeros of the order-parameter field, which could, in turn, be mapped onto the zeros of a Gaussian auxiliary field. The point defect charge density correlation function G_ρ was determined using this technique in terms of the constrained quantity f. Since f was not determined in the calculation, it was assumed that $f=f_{\rm OP}$ in order to make further progress. For large defect separations, G_ρ was found to agree with numerical simulations [12] and experiments [13] relevant to the case $n=2$. However, for $n=2$ the theory produced an unphysical divergence in G_ρ at short-scaled distances x due to a nonanalytic piece in auxiliary field correlation function $f_{\rm OP}$ at small x. This nonanalytic piece occurs in the most elementary self-consistent theory for $f_{\rm OP}$ [7] but Mazenko and Wickham [2] have since shown that one can construct the theory so that $f_{\rm OP}$ is analytic in x. This development highlights the difference between the order-parameter correlation function, whose short distance non-analyticities are essential and lead to the observed generalized Porod's law [14] for the structure factor, and f, which must be smooth in order to have sensible theories of defect position and velocity [15] correlations. The f obtained from OJK is smooth.

The approach we take in this paper is distinct and independent from that used by OJK or that developed in [6]. The technique used here is directly based on considerations of topological charge conservation and is less directly based on the TDGL model. This leads to the important difference that we treat quantities that are constrained to be evaluated at the defect core.

The system studied here has a defect dynamics generated by the TDGL model for a nonconserved n-component vector order parameter $\vec{\psi}(\vec{r},t)$:

$$\frac{\partial\vec{\psi}}{\partial t}=\vec{K}\equiv-\Gamma\frac{\delta F}{\delta\vec{\psi}}, \tag{1}$$

where Γ is a kinetic coefficient, and F is a Ginzburg-Landau effective free energy assumed to be of the form

$$F=\int d^dr\left(\frac{c}{2}(\nabla\vec{\psi})^2+V(|\vec{\psi}|)\right). \tag{2}$$

The coefficient c is positive and the potential V is assumed to be of the $O(n)$-symmetric, degenerate double-well form. We assume that the quench is from an initial high-temperature disordered state to zero temperature so the usual noise term in Eq. (1) is set to zero.

In previous work [7] on the order-parameter correlation function progress was made by mapping the order parameter $\vec{\psi}$ onto an auxiliary field $\vec{m}$, with the requirement that *away* from the defect cores

$$\vec{\psi}=\psi_0\hat{m}, \tag{3}$$

where ψ_0 is the magnitude of $\vec{\psi}$ in the ordered phase. Physically, we interpret $\vec{m}$ to be the position relative to the nearest defect and expect that *near* the defect cores

$$\vec{\psi}=a\vec{m}+b\vec{m}(\vec{m})^2+\cdots \tag{4}$$

where the coefficients a and b depend on the details of the potential V. Equations (3) and (4) represent topological charge ±1 defects, which have the lowest energy and dominate the late-time regime [16]. In the theory for order-parameter correlations [7] property (3) is crucial, whereas, in the theory of defect motion presented here property (4) is relevant since we always work near the defect cores.

In the simplest models [6,7], considered here, the auxiliary field $\vec{m}$, defined everywhere, is assumed to be a Gaussian field with a normalized correlation function f defined as

$$\delta_{\mu\nu}f(12)=\frac{\langle m_\mu(1)m_\nu(2)\rangle}{\sqrt{S_0(1)S_0(2)}} \tag{5}$$

with $\delta_{\mu\nu}S_0(1)=\langle m_\mu(1)m_\nu(1)\rangle$. Here we use the shorthand $m_\mu(1)=m_\mu(\vec{r}_1,t_1)$. If f is determined within a theory of the order-parameter correlation function [6,7] it is referred to as $f_{\rm OP}$. However, if $(\vec{r}_1,t_1)$ and $(\vec{r}_2,t_2)$ are constrained to be the coordinates of defect cores f is the constrained quantity mentioned in the first paragraph, which is used exclusively in the calculations below. Near a defect core the linear part of Eq. (4) allows one to identify the order-parameter correlation function with the auxiliary field correlation function f.

It is well established that for late times t following the quench the dynamics obey scaling and the system can be described in terms of a single growing length $L(t)$, which is characteristic of the spacing between defects. For a nonconserved order parameter $L(t)\sim t^{1/2}$ at late times. Since we interpret $|\vec{m}|$ to be the distance to the nearest defect we expect $|\vec{m}|\sim L$ on average. At equal times ($t_1=t_2=t$) in the scaling regime the auxiliary field correlation function can be written solely in terms of the scaled length $x=|\vec{r}_2-\vec{r}_1|/L(t)$. Hence $f(12)=f(x)$.

The emphasis in this paper is on defect densities like the charge density for point defects, given in terms of the order parameter by [11]

$$\rho=\delta(\vec{\psi})\mathcal{D}, \tag{6}$$

where the Jacobian associated with the change of variables from the set of defect positions to the field $\vec{\psi}$ is defined by

$$\mathcal{D}=\frac{1}{n!}\epsilon_{\mu_1\mu_2\cdots\mu_n}\epsilon_{\nu_1\nu_2\cdots\nu_n}\nabla_{\mu_1}\psi_{\nu_1}\nabla_{\mu_2}\psi_{\nu_2}\cdots\nabla_{\mu_n}\psi_{\nu_n}. \tag{7}$$

$\epsilon_{\mu_1\mu_2\cdots\mu_n}$ is the n-dimensional fully antisymmetric tensor and summation over repeated indices in Eq. (7) is implied.

It was shown in a direct manner in [5] that ρ satisfies the continuity equation for topological charge:

$$\frac{\partial\rho}{\partial t}=\nabla_\alpha[\,\delta(\vec{\psi})J^{(K)}_\alpha], \tag{8}$$

where the current $J^{(K)}_\alpha$ is defined as

$$J^{(K)}_\alpha=\frac{1}{(n-1)!}\epsilon_{\alpha\mu_2\cdots\mu_n}\epsilon_{\nu_1\nu_2\cdots\nu_n}K_{\nu_1}\nabla_{\mu_2}\psi_{\nu_2}\cdots\nabla_{\mu_n}\psi_{\nu_n}. \tag{9}$$

The derivation of Eq. (8) is independent of the details of the TDGL model, except that Eq. (1) is first order in time. Since $\vec{J}^{(K)}$ is multiplied by the defect-locating δ function we can replace $\vec{K}$ in $\vec{J}^{(K)}$ by the part of $\vec{K}$ that does not vanish as $\vec{\psi}\to0$. For a nonconserved order parameter this means that we can set $\vec{K}=\Gamma c\nabla^2\vec{\psi}$ in Eq. (8). Equation (8) is in the standard form of a continuity equation, allowing us to identify the vortex velocity field as

$$v_\alpha=-\frac{J^{(K)}_\alpha}{\mathcal{D}}, \tag{10}$$

where it is assumed that the velocity field is used inside expressions multiplied by the vortex-locating δ function.

For string defects the charge density is a vector given by [11]

$$\rho_\alpha=\delta(\vec{\psi})\omega_\alpha \tag{11}$$

with

$$\omega_\alpha=\frac{1}{n!}\epsilon_{\alpha\mu_1\mu_2\cdots\mu_n}\epsilon_{\nu_1\nu_2\cdots\nu_n}\nabla_{\mu_1}\psi_{\nu_1}\nabla_{\mu_2}\psi_{\nu_2}\cdots\nabla_{\mu_n}\psi_{\nu_n}. \tag{12}$$

As in [5] one can obtain the continuity equation satisfied by ρ_α by combining the two identities

$$\dot{\omega}_\alpha=\nabla_\beta J^{(K)}_{\alpha\beta} \tag{13}$$

and

$$K_\gamma \omega_\alpha = J^{(K)}_{\alpha\beta} \nabla_\beta \psi_\gamma \tag{14}$$

to obtain

$$\frac{\partial \rho_\alpha}{\partial t} = \nabla_\beta [\delta(\vec{\psi}) J^{(K)}_{\alpha\beta}]. \tag{15}$$

The string defect current tensor $J^{(K)}_{\alpha\beta}$ is defined as

$$J^{(K)}_{\alpha\beta} = \frac{1}{(n-1)!} \epsilon_{\alpha\beta\mu_2\cdots\mu_n} \epsilon_{\nu_1\nu_2\cdots\nu_n} K_{\nu_1} \nabla_{\mu_2}\psi_{\nu_2} \cdots \nabla_{\mu_n}\psi_{\nu_n}. \tag{16}$$

For the important case of $n=2$, $d=3$ we can write

$$J^{(K)}_{\alpha\beta} = v_\alpha \omega_\beta - v_\beta \omega_\alpha \tag{17}$$

and identify the string velocity as

$$\vec{v} = \frac{1}{\omega^2}(\vec{\omega} \times \vec{g}), \tag{18}$$

where $\vec{g} = \epsilon_{\nu_1\nu_2} K_{\nu_1} \vec{\nabla} \psi_{\nu_2}$ [17].

We use the continuity equation for topological charge to determine the auxiliary field correlation function. We begin by examining point defects and require that the exact equation

$$\frac{\partial}{\partial t}\langle \rho(1)\rho(2)\rangle = \nabla^{(1)}_\beta \langle \delta[\vec{\psi}(1)] J^{(K)}_\beta(1)\rho(2)\rangle + \nabla^{(2)}_\beta \langle \rho(1)\delta[\vec{\psi}(2)] J^{(K)}_\beta(2)\rangle \tag{19}$$

be satisfied at equal times. The presence of the δ functions in Eq. (19) enables us to use relation (4) to replace $\vec{\psi}$ with the Gaussian auxiliary field $\vec{m}$ in Eq. (19). The left-hand side of Eq. (19) involves the point defect charge density correlation function defined by

$$G_\rho(12) = \langle \rho(1)\rho(2)\rangle. \tag{20}$$

As shown in [1], G_ρ factors into a product of Gaussian averages, which can be evaluated in terms of the constrained f, Eq. (5), using standard methods. In the scaling regime G_ρ has the form

$$G_\rho(12) = \frac{g(x)}{L^{2n}} \tag{21}$$

with $g(x)$ given by

$$g(x) = n! \left[\frac{h(x)}{x}\right]^{n-1} \frac{\partial h(x)}{\partial x}, \tag{22}$$

and h given by

$$h = -\frac{\gamma f'}{2\pi} \tag{23}$$

with $\gamma = 1/\sqrt{1-f^2}$. In the earlier calculation [1] the function f was undetermined at this point and the assumption was made that $f = f_{\rm OP}$, which was determined from theories of the order parameter [6,7]. However, here we can use Eq. (19) to determine f, the constrained quantity, directly. It is clear that the left-hand side of Eq. (19) is a complicated nonlinear function of f and its derivatives. The right-hand side of Eq. (19) involves the evaluation of

$$N_\beta(12) = \langle \delta[\vec{m}(1)] \mathcal{D}(1) \delta[\vec{m}(2)] J^{(K)}_\beta(2)\rangle, \tag{24}$$

which, like the evaluation of G_ρ, factors into products of averages over the n separate components of $\vec{m}$. We easily find

$$N_\beta(12) = n!\Gamma c B(A)^{n-1} \hat{x}_\beta, \tag{25}$$

where, in the scaling regime, A is given by

$$A = \frac{1}{L^2}\frac{h}{x} \tag{26}$$

and B is

$$B = \frac{\widetilde{B}}{L^3} \tag{27}$$

with

$$2\pi \widetilde{B} = \frac{d}{dx}\left[\gamma\left(\nabla^2 f + \frac{nS^{(2)}}{\sigma} f\right)\right]. \tag{28}$$

We have defined $S^{(2)} = \Sigma_{\alpha\beta}\langle [\nabla_\alpha m_\beta]^2\rangle / n^2$ and $\sigma = S_0/L^2$, which are both constants at late times.

Having compiled these results, it is easy to see that Eq. (19) reduces, in the scaling regime, to

$$\mu \frac{d}{dx}[h^n + x h^{n-1} h'] = \frac{d}{dx}[\widetilde{B} h^{n-1}], \tag{29}$$

where we have defined the constant

$$\mu = \frac{L\dot{L}}{2\Gamma c}. \tag{30}$$

Equation (29) can be integrated to give

$$\mu \frac{d}{dx}(xh) = \widetilde{B}, \tag{31}$$

with the integration constant determined to be zero by the condition that f and h vanish as $x \to \infty$. Equation (28) shows us that $\widetilde{B}$ is the derivative of a quantity that vanishes at $x \to \infty$. Thus we can integrate Eq. (31) yet again, and use Eq. (23), to obtain the remarkable final result:

$$-\mu x f' = \nabla^2 f + \frac{nS^{(2)}}{\sigma} f, \tag{32}$$

which is linear in f.

For string defects, the analogous calculation involves evaluating the averages in

$$\frac{\partial}{\partial t}\langle \rho_\alpha(1)\rho_\beta(2)\rangle = \nabla^{(1)}_\gamma \langle \delta[\vec{\psi}(1)] J^{(K)}_{\alpha\gamma}(1)\rho_\beta(2)\rangle + \nabla^{(2)}_\gamma \langle \rho_\alpha(1)\delta[\vec{\psi}(2)] J^{(K)}_{\beta\gamma}(2)\rangle. \tag{33}$$

The string charge density correlation function

$$G_{\alpha\beta}(12)=\langle\rho_\alpha(1)\rho_\beta(2)\rangle \tag{34}$$

was first worked out by Liu and Mazenko [1] with the scaling result

$$G_{\alpha\beta}(12)=\frac{1}{L^{2n}}[G_T(x)(\delta_{\alpha\beta}-\hat{x}_\alpha\hat{x}_\beta)+G_L(x)\hat{x}_\alpha\hat{x}_\beta] \tag{35}$$

where the transverse function is

$$G_T(x)=n!\left(\frac{h}{x}\right)^{n-1}\frac{\partial h}{\partial x} \tag{36}$$

and the longitudinal function is

$$G_L(x)=n!\left(\frac{h}{x}\right)^{n}. \tag{37}$$

h is defined in Eq. (23). We evaluate the average appearing on the right-hand side of Eq. (33) using the same techniques that were used in the point defect case and easily obtain

$$\langle\delta[\vec{m}(1)]J^{(K)}_{\alpha\gamma}(1)\rho_\beta(2)\rangle=n!\Gamma cB(A)^{n-1}[\hat{x}_\alpha\delta_{\beta\gamma}-\hat{x}_\gamma\delta_{\alpha\beta}], \tag{38}$$

where A is defined in Eq. (26) and B in Eq. (27). Substitution of the results (35) and (38) into Eq. (33) leads to separate equations for the longitudinal and transverse components. Both equations reduce to Eq. (32). Thus the same linear equation determines f for both point and string defects.

The solution of Eq. (32) is of the OJK form,

$$f(x)=\exp-\frac{\mu}{2}x^2, \tag{39}$$

where we have used the relation

$$\frac{nS^{(2)}}{\sigma}=(-\nabla^2 f)|_{x=0}=n\mu. \tag{40}$$

The constant μ is fixed through a choice of the length scale L, since $L=\sqrt{4\Gamma c\mu}t^{1/2}$. Since Eq. (32) is linear, the probability distribution governing the auxiliary field is Gaussian for all times. We are therefore lead directly, without any approximation except that the order parameter field can be treated as Gaussian near its zeros, to a self-consistent result.

It should be noted that at leading order in a systematic large-N approximation scheme for a color index N Bray and Humayun [10] were able to recover the previously *ad hoc* Oono-Puri [9] extension of OJK, which, in turn, gives *exactly* Eq. (32). In the development here, Eq. (32) arises without the need for any such approximations.

This work emphasizes the distinction between theories of the order-parameter correlation function, such as in Ref. [6], and theories concerning defect correlation functions, where it appears one can self-consistently use the Gaussian closure approximation if one uses the OJK form for the auxiliary field correlation function. The theory of order-parameter correlations does a superior job determining the nonequilibrium exponent governing the decay of two-time autocorrelation functions [7,18], but the use of the theory presented here for defect correlations, with its smooth OJK-like auxiliary field, avoids the difficulties due to nonanalyticities at small x. The reconciliation between theories of the order-parameter correlation function and the theory presented here, involving defect densities, is an interesting area of current research.

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