Defect-defect correlation in the dynamics of first-order phase transitions

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We investigate the defect structures evolving after a temperature quench from a disordered phase into an ordered phase for systems with O(n) symmetry. Various defect-defect correlation functions are calculated. These quantities exhibit scaling behavior as well as interesting short-distance behavior which are sensitive to the structure of the theory.

I. INTRODUCTION

The study of the growth kinetics of systems subjected to rapid temperature quenches¹⁻⁷ has recently been extended to include systems with more complex order parameter symmetries.⁸⁻¹⁴ In particular there has been progress on the study of the *n*-vector model with nonconserved Langevin dynamics. Results for the order parameter correlation functions satisfy scaling for all values of nand show nonanalytic behavior for short-scaled distances which weakens as n increases.¹⁰⁻¹² There is, however, no dramatic variation of the scaling function as a function of *n* and the growth law follows a $t^{1/2}$ time dependence for all values of n. There are, on the other hand, other quantities of interest in these systems which we do expect to vary strongly with n. In particular the topological defect structures, which are the disordering agents controlling the growth of ordering in these unstable systems, should show a strong variation with n. In this paper we study the statistical properties of and the correlations among these defects. In particular, we calculate here the defect densities and various defect-defect correlation functions for different n and dimensionality d for the same TDGL model studied in Ref. 11 and defined below. It turns out that these correlation functions depend sensitively on the detailed structure of a theory. Hence they are more suitable than the usual order-parameter correlation function to be compared with numerical simulations and experiments, since one may be able to discriminate among different theories. These defect correlations may even turn out to be easily measurable by digitization methods since only the positions of the defects are involved. We show that some of our results can be directly compared with numerical simulations, and hopefully these and other results can be checked by future experiments.

In previous work¹¹ we discussed the development of a quantitative method for treating growth kinetics of the order parameter field $\psi(\mathbf{r},t)$. Here we focus more closely on the defects associated with this field. Let us begin by briefly reviewing the nature of the defects for the O(n) symmetric *n*-vector model. For the scalar case, n = 1, the defects are domain walls which are points for d = 1, lines for d = 2, planes for d = 3, etc. More generally, for n = d one has point defects. This leads to vortices for n = d = 2 and monopoles for n = d = 3. For n = d - 1 one generates string-type defects.

In the case of point defects (n = d), it is clear that we can introduce a defect density

$$\rho(\mathbf{r},t) = \sum_{\alpha} q_{\alpha} \delta(\mathbf{r} - \mathbf{x}_{\alpha}(t)) , \qquad (1.1)$$

where $\mathbf{x}_{\alpha}(t)$ is the position of the α th point defect at time t and with a charge q_{α} . For the case n = d - 1, where one has strings, one can define the defect line density

$$\boldsymbol{\rho}(\mathbf{r},t) = \sum_{\alpha} \int ds \frac{d\mathbf{x}_{\alpha}}{ds} \delta(\mathbf{r} - \mathbf{x}_{\alpha}(s,t)) , \qquad (1.2)$$

where s parametrizes the string along its curve and dx_{α}/ds can be chosen to point in the direction of positive winding number for the singularity. In this paper we are primarily concerned with the defect-correlation functions

$$G(\mathbf{r},t) = \langle \rho(\mathbf{r},t)\rho(0,t) \rangle \tag{1.3}$$

and

$$G_{ij}(\mathbf{r},t) = \langle \rho_i(\mathbf{r},t)\rho_j(0,t) \rangle .$$
(1.4)

The determination of these quantities is a formidable task but can be carried out via the following steps: (i) relate the densities ρ and ρ to zeros in the order parameter field ψ ; (ii) express, under the appropriate circumstances to be discussed in detail below, ψ in terms of an *n*component auxiliary field **m**. **m** has the same zeros as ψ but, unlike ψ , can be treated as a Gaussian field; (iii) reexpress ρ and ρ in terms of **m**; (iv) since **m** is a Gaussian field we can then explicitly evaluate G and G_{ij} in terms of the variances of **m**:

$$C_0(\mathbf{r},t)\delta_{ii} \equiv \langle m_i(\mathbf{r},t)m_i(0,t) \rangle . \tag{1.5}$$

We summarize here the main results of this calculation. For the case n = d, we find that G is of the form

$$G(\mathbf{r},t) = n_0(t)\delta(\mathbf{r}) + g(\mathbf{r},t) , \qquad (1.6)$$

where the δ -function contribution arises from the correlation of point defects at the same position. Clearly $n_0(t)$ is the total (unsigned) number density of defects at time t. The correlation function for different defects is given by

$$g(\mathbf{r},t) = n! \left[\frac{h}{r}\right]^{n-1} \frac{\partial h}{\partial r} , \qquad (1.7)$$

where

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$$h(\mathbf{r},t) = -\frac{1}{2\pi} \frac{\partial f(\mathbf{r},t)/\partial \mathbf{r}}{\sqrt{1-f^2}}$$
(1.8)

and f is the normalized variance of \mathbf{m} :

$$f(\mathbf{r},t) = \frac{C_0(\mathbf{r},t)}{C_0(0,t)} .$$
(1.9)

The density of defects can be obtained from the "charge" conservation law satisfied by ρ and is given by

$$n_{0}(t) = -\int d\mathbf{r} g(\mathbf{r}, t)$$

$$= \frac{n! [-f''(0, t)]^{n/2}}{2^{n} \pi^{n/2} \Gamma(1 + n/2)} . \qquad (1.10)$$

For the case n = d - 1 we obtain

$$G_{ij}(\mathbf{r},t) = G_L(\mathbf{r},t) \hat{\mathbf{r}}_i \hat{\mathbf{r}}_j + G_T(\mathbf{r},t) (\delta_{ij} - \hat{\mathbf{r}}_i \hat{\mathbf{r}}_j) , \qquad (1.11)$$

where the longitudinal part is given by

$$G_L(\mathbf{r},t) = n! \left[\frac{h}{r}\right]^n \tag{1.12}$$

and the transverse part takes the identical form as $g(\mathbf{r}, t)$:

$$G_T(\mathbf{r},t) = n! \left[\frac{h}{r}\right]^{n-1} \frac{\partial h}{\partial r} . \qquad (1.13)$$

In both cases it is easy to verify the overall charge neutrality:

$$\int G(\mathbf{r},t)d\mathbf{r}=0, \qquad (1.14)$$

$$\int G_{ij}(\mathbf{r},t) d\mathbf{r} = 0 . \qquad (1.15)$$

These results follow rather generally as long as the zeros defining the defects can be associated with a Gaussian field. Similar results have been previously derived by Halperin in the equilibrium context.¹⁵ In the specific case of growth kinetics, one must then identify the function $f(\mathbf{r},t)$, which appears in our results. In our work in Ref. 11, we self-consistently evaluated $f(\mathbf{r},t)$ for the *n*-vector model and details will be given in sections below. Here we use the main property of f that it satisfies the similarity scaling relation

$$f(\mathbf{r},t) = f(\mathbf{r}/L(t)) \tag{1.16}$$

in the long-time limit where the characteristic length $L(t) \sim t^{1/2}$ for a nonconserved TDGL *n*-vector model. This relation allows us to extract the overall time dependence of our defect-correlation functions when expressed in terms of the scaled length $\mathbf{x} \equiv \mathbf{r}/L(t)$. For n = d,

$$g(\mathbf{x},t) = n! \left[\frac{\tilde{h}}{x}\right]^{n-1} \frac{\partial \tilde{h}}{\partial x} \frac{1}{L^{2n}(t)} , \qquad (1.17)$$

where \tilde{h} is the dimensionless quantity

$$\tilde{h}(x) = \frac{-f'(x)}{2\pi\sqrt{1-f^2}} , \qquad (1.18)$$

while for n = d - 1 we have

$$G_L(\mathbf{x},t) = n! \left(\frac{\tilde{h}}{x}\right)^n \frac{1}{L^{2n}(t)}$$
(1.19)

and

$$G_T(\mathbf{x},t) = \frac{(n-1)!}{x^{n-1}} \frac{\partial \tilde{h}^n}{\partial x} \frac{1}{L^{2n}(t)} . \qquad (1.20)$$

Thus all of the correlation functions fall off with time as $L^{-2n} \sim t^{-n}$ and the coefficients are scaling functions providing information about the spatial correlations among defects. These depend rather sensitively on the precise nature of f(x) as we shall discuss in detail below.

In the next section we discuss the basic assumptions leading to the results (1.7) and (1.11) for G and G_{ij} . In Sec. III we consider the scalar (n = 1) case where we can establish some interesting connections between $G_{ij}(\mathbf{r}, t)$ and the order-parameter scaling function. In Secs. IV and V, the derivations of the results for G and G_{ij} are provided in detail. We also examine the forms of the associated scaling functions which follow from the theory we developed previously.

II. DEFECT STRUCTURE AND DENSITIES

A. Model

The fundamental model of interest here is the timedependent Ginzburg-Landau (TDGL) model with a *n*vector order parameter $\psi(\mathbf{r}, t)$, governed by the Langevin equation,

$$\frac{\partial \boldsymbol{\psi}(\mathbf{r},t)}{\partial t} = -\Gamma \frac{\delta F[\boldsymbol{\psi}]}{\delta \boldsymbol{\psi}} + \boldsymbol{\eta}(\mathbf{r},t) , \qquad (2.1)$$

where the driving free energy is of the form

$$F[\boldsymbol{\psi}(\mathbf{r},t)] = \int d\mathbf{r} \left[\frac{1}{2} (\nabla \boldsymbol{\psi})^2 + V(\boldsymbol{\psi})\right]$$
(2.2)

and $V(\psi)$ has the "Mexican hat" form. The Gaussian thermal noise η has zero mean and satisfies

$$\langle \eta_i(\mathbf{r},t)\eta_j(\mathbf{r}',t')\rangle = k_B T \Gamma \delta_{ij} \delta(\mathbf{r}-\mathbf{r}')\delta(t-t')$$
, (2.3)

where T is the temperature and Γ is a kinetic coefficient.

We assume that the system is prepared in an initially disordered equilibrium state at high temperatures with

$$\langle \boldsymbol{\psi}(\mathbf{r},t) \rangle = 0$$
, (2.4)

$$\langle \psi_i(\mathbf{r},t)\psi_j(\mathbf{r}',t')\rangle = \delta_{ij}\epsilon_I \delta(\mathbf{r}-\mathbf{r}')$$
 (2.5)

At time t=0 the system is quenched such that it is governed by (2.1) for t > 0. We assume that the final temperature T is below the critical temperature. Indeed we will assume here that the quench is to T=0. Under these circumstances the system will develop ordered regions which grow indefinitely larger with time. In the late stages of the ordering, growth is controlled by the motion and annihilation of strongly interacting low-energy defects. These defects are point- and stringlike in the two cases n=d and n=d-1, respectively. The field configuration associated with an isolated defect is given by the nonuniform solution of the classical equation

5964

$$\nabla^2 \boldsymbol{\psi}_c - \boldsymbol{V}'(\boldsymbol{\psi}_c) = 0 \ . \tag{2.6}$$

We assume for the cases treated here that late stage coarsening involves only those defects with the lowest energy and thus those with topological charge ± 1 . Solutions of this type take the form

$$\boldsymbol{\psi}_{c}(\boldsymbol{\rho}) = \boldsymbol{A}(\boldsymbol{\rho})\boldsymbol{\hat{\rho}} , \qquad (2.7)$$

where the amplitude $A(\rho)$ vanishes at the defect core and satisfies

$$\nabla_{\rho}^{2}A - \frac{(n-1)}{\rho^{2}}A - \frac{\partial V[A]}{\partial A} = 0$$
(2.8)

and ρ is an *n*-dimensional coordinate measured from the defect core.

B. Separation of fields

The key assumption made in the development of the analytic theory in Refs. 6, 7, and 11 is that the order parameter field can be decomposed into a sum of two fields:

$$\boldsymbol{\psi}(\mathbf{r},t) = \boldsymbol{\sigma}[\mathbf{m}(\mathbf{r},t)] + \boldsymbol{\phi}(\mathbf{r},t) , \qquad (2.9)$$

where σ has the same form as the classical defect solution except the coordinate variable ρ is replaced by an auxiliary field **m**. Thus the field $\mathbf{m}(\mathbf{r},t)$ has the physically appealing interpretation of the distance from the point **r** to the nearest defect. In the case of interest here where the relevant defects are unit charge vortices we have

$$\boldsymbol{\sigma}(\mathbf{m}) = \boldsymbol{A}(\boldsymbol{m}) \mathbf{\hat{m}} . \qquad (2.10)$$

The field ϕ in (2.9) represents the fluctuations in ψ about its ordered component. As discussed in detail in Ref. 6 for the scalar case, ϕ is not properly defined until we specify the statistical distribution governing the field m. We are free to choose any statistical distribution we desire. However, the selected distribution will influence the statistical properties of the field ϕ . Thus without loss of generality we can choose m to be governed by a Gaussian distribution and then investigate the resulting behavior of the field ϕ . It was shown in the scalar case for a nonconserved order parameter that in the scaling regime the field ϕ could be neglected in the computation of the order-parameter scaling function. In this case one finds that the field σ and ϕ decouple in the scaling regime. In Ref. 11 we assumed this decoupling from the beginning. One must be careful about this assumption. In the case of a conserved scalar order parameter, in order to allow for diffusive processes which lead to an interaction between separate interfaces, one must allow for an interaction between the σ and ϕ fields.¹⁶ Henceforth, unless stated otherwise, we assume here that in treating the late stages we can ignore the ϕ variable and treat m as a Gaussian variable.

C. Defect fields

We next consider the appropriate form for the defect densities when expressed in terms of the fundamentalorder parameter field $\psi(\mathbf{r},t)$. In the case n=d, this analysis has been carried out by Halperin.¹⁵ The first ingredient is the rather obvious result

$$\sum_{\alpha} \delta(\mathbf{r} - \mathbf{x}_{\alpha}(t)) = \delta(\boldsymbol{\psi}(\mathbf{r}, t)) |\det \partial \boldsymbol{\psi}| , \qquad (2.11)$$

where the second factor on the right-hand side is just the Jacobian of the transformation from the variable ψ to r. This is combined with the less obvious result

$$q_{\alpha} = \operatorname{sgn}(\operatorname{det}\partial \psi)_{\mathbf{r}=\mathbf{x}}$$
(2.12)

to give

$$\rho(\mathbf{r},t) = \sum_{\alpha} q_{\alpha} \delta(\mathbf{r} - \mathbf{x}_{\alpha}) = \delta(\boldsymbol{\psi}) \det(\partial \boldsymbol{\psi}) . \qquad (2.13)$$

Halperin also showed for the case n = d - 1 that

$$\rho_i(\mathbf{r},t) = \delta(\boldsymbol{\psi}) \epsilon_{ii_1 i_2 \cdots i_n} \partial_{i_1} \psi_1 \partial_{i_2} \psi_2 \cdots \partial_{i_n} \psi_n , \qquad (2.14)$$

where ϵ is the *d*-dimensional Levi-Civita antisymmetric tensor and summation is implied over the repeated indices.

The important assumption we make here is that, for long times and in the scaling regime, we can write

$$\boldsymbol{\psi}(\mathbf{r},t) = \boldsymbol{\sigma}[\mathbf{m}(\mathbf{r},t)] \tag{2.15}$$

and require that the zeros of ψ coincide with the zeros of **m**. It is then clear that we can replace ψ by **m** in the expressions for the defect density and obtain

$$\rho(\mathbf{r},t) = \delta[\mathbf{m}(\mathbf{r},t)] \det(\partial \mathbf{m})$$
(2.16)

for the case n = d and

$$\rho_i(\mathbf{r},t) = \delta[\mathbf{m}(\mathbf{r},t)] \epsilon_{ii_1i_2\cdots i_n} \partial_{i_1}m_1 \partial_{i_2}m_2 \partial_{i_n}m_n \quad (2.17)$$

for the case n = d - 1.

In the scalar case (n = 1), it is more convenient to introduce a density

$$\rho_i^{s}(\mathbf{r},t) = \delta(\psi)\partial_i\psi(\mathbf{r},t) = \delta(m)\partial_im(\mathbf{r},t)$$
(2.18)

which measures the amount of interface and its local orientation. Thus ρ^s is perpendicular to a domain "wall." For n = d = 1, ρ^s is related to ρ by

$$\rho^{s}(\mathbf{r},t) = \rho(\mathbf{r},t) , \qquad (2.19)$$

while for n = 1, d = 2,

$$\rho_x^s(\mathbf{r},t) = -\rho_y(\mathbf{r},t), \quad \rho_y^s(\mathbf{r},t) = \rho_x(\mathbf{r},t) . \quad (2.20)$$

In the next three sections we undertake the study of $G(\mathbf{r},t)$, $G_{ii}(\mathbf{r},t)$, as well as

$$G_{ij}^{s}(\mathbf{r},t) = \langle \rho_{i}^{s}(\mathbf{r},t) \rho_{j}^{s}(0,t) \rangle . \qquad (2.21)$$

We start with G_{ij}^s since the analysis is somewhat simpler.

III. THE SCALAR CASE

In discussing the scalar case it is useful to concentrate first on the total interfacial area density

$$n_0^{s}(\mathbf{r},t) = \langle \delta[m(\mathbf{r},t)] | \partial m(\mathbf{r},t) | \rangle$$
(3.1)

which measures the amount of interface independent of orientation. To calculate this quantity we take advantage of the identity

$$|a|^{-1} = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} \exp(-a^2 x^2/2)$$
 (3.2)

to write

$$n_{0}^{s}(t) = \left\langle \delta(m) \frac{(\partial m)^{2}}{|\partial m|} \right\rangle$$
$$= -\int \frac{dx}{\sqrt{2\pi}x} \frac{\partial}{\partial x} \left\langle \delta(m) e^{-(\partial m)^{2}x^{2}/2} \right\rangle .$$
(3.3)

In evaluating Gaussian averages over m we will repeatedly use the fundamental result

$$\left\langle \exp \int d1 \sum_{i=1}^{n} H_{i}(1)m_{i}(1) \right\rangle$$

= $\exp \frac{1}{2} \sum_{i,j} \int d1 d2 H_{i}(1)H_{j}(2)\delta_{ij}C_{0}(12) , \quad (3.4)$

where we use the notation $1 = (\mathbf{r}_1, t_1)$ for convenience. It is also assumed that the systems are isotropic as well as homogeneous and

$$\delta_{ij}C_0(|\mathbf{r}_1 - \mathbf{r}_2|, t_1, t_2) = \langle m_i(\mathbf{r}_1, t_1)m_j(\mathbf{r}_2, t_2) \rangle .$$
(3.5)

We can put the average occurring in (3.3) into the form given by (3.4) by using the standard integral representation for the δ function and the identity

$$\exp(-\mathbf{a}^2/2) = \int \frac{d^d \mathbf{y}}{(2\pi)^{d/2}} \exp(-y^2/2 + i\mathbf{a} \cdot \mathbf{y}) . \quad (3.6)$$

We obtain

This average is of the standard form (3.4) with

$$H(\mathbf{r}_1, t_1) = (ik + ix \mathbf{y} \cdot \nabla_{\mathbf{r}}) \delta(\mathbf{r} - \mathbf{r}_1) \delta(t - t_1) . \qquad (3.8)$$

 $n_0^{s}(t) = -\int \frac{dx}{\sqrt{2\pi}x} \frac{\partial}{\partial x} \int \frac{d^d \mathbf{y}}{(2\pi)^{d/2}} e^{-y^2/2} \int \frac{dk}{2\pi} \langle e^{ikm + ix\partial m \cdot \mathbf{y}} \rangle .$

It is then easy to show that

$$\langle e^{ikm + ixy \cdot \partial m} \rangle = \exp{-\frac{1}{2} [k^2 S_0(t) + x^2 y^2 S_2(t)]},$$
 (3.9)

where

$$S_0(t) \equiv \langle m^2(\mathbf{r}, t) \rangle = C_0(0, t) ,$$
 (3.10)

$$S_{2}(t) \equiv \frac{1}{d} \left\langle \left[\partial m(\mathbf{r},t) \right]^{2} \right\rangle = -C_{0}^{\prime\prime}(r,t) \bigg|_{r=0}, \qquad (3.11)$$

and we have used the result

$$\langle [\partial_i m(\mathbf{r},t)]m(\mathbf{r},t) \rangle = 0$$
. (3.12)

The integration over k and y in (3.7) can then be carried out with the result¹⁷

$$n_{0}^{s}(t) = -\frac{1}{2\pi\sqrt{S_{0}}} \int \frac{dx}{x} \frac{\partial}{\partial x} \frac{1}{(1+x^{2}S_{2})^{d/2}}$$
$$= \frac{\Gamma[(d+1)/2]}{\Gamma(d/2)} \left[\frac{S_{2}}{\pi S_{0}}\right]^{1/2}.$$
(3.13)

Since $S_0(t) \sim t$ and $S_2(t) \rightarrow \frac{1}{2}$ for large t, we see that $n_0^s(t) \sim t^{-1/2}$ for all d.

We turn next to the correlation function G_{ij}^s defined by (2.21) and given more explicitly by

$$G_{ij}^{s}(12) = \left\langle \delta[m(1)]\partial_{i}m(1)\delta[m(2)]\partial_{j}m(2) \right\rangle . \tag{3.14}$$

Because the average over m is Gaussian we have the general theorem

$$\langle m_i(1)B[m] \rangle = \int d\overline{1} C_0(1\overline{1}) \left\langle \frac{\delta B[m]}{\delta m_i(\overline{1})} \right\rangle.$$
 (3.15)

Using this general result we easily reduce (3.14) to

$$G_{ij}^{s}(12) = \partial_{i}^{1}C_{0}(12)\partial_{j}^{2}C_{0}(12)\langle \delta'[m(1)]\delta'[m(2)] \rangle + \partial_{i}^{1}\partial_{j}^{2}C_{0}(12)\langle \delta[m(1)]\delta[m(2)] \rangle .$$
(3.16)

Evaluation of the remaining averages is straightforward using the techniques already developed. We obtain

$$\langle \delta[m(1)]\delta[m(2)] \rangle = \int \frac{dk_1 dk_2}{4\pi^2} \langle e^{ik_1 m(1) + ik_2 m(2)} \rangle$$
$$= \frac{\gamma(12)}{2\pi \sqrt{S_0(1)S_0(2)}}$$
(3.17)

and

$$\langle \delta'[m(1)]\delta'[m(2)]\rangle = \frac{\partial}{\partial C_0(12)} \langle \delta[m(1)]\delta[m(2)]\rangle$$

$$=\frac{\gamma^{3}(12)f(12)}{\sqrt{S_{0}(1)S_{0}(2)}},\qquad(3.18)$$

where we have defined

$$\gamma(12) = [1 - f^2(12)]^{-1/2} \tag{3.19}$$

and

$$f(12) = \frac{C_0(12)}{\sqrt{S_0(1)S_0(2)}} . \tag{3.20}$$

Combining these results gives

$$G_{ij}^{s}(12) = \frac{1}{2\pi} \left[(\partial_i^1 \partial_j^2 f) \gamma + (\partial_i^1 f) (\partial_j^2 f) f \gamma^3 \right] .$$
(3.21)

Using the isotropic nature of the problem

$$f(12) = f(r, t_1, t_2) , \qquad (3.22)$$

where $r = |\mathbf{r}_1 - \mathbf{r}_2|$ we can write

$$G_{ij}^{s}(\mathbf{r},t_{1},t_{2}) = G_{L}^{s} \hat{\mathbf{r}}_{i} \hat{\mathbf{r}}_{j} + G_{T}^{s} (\delta_{ij} - \hat{\mathbf{r}}_{i} \hat{\mathbf{r}}_{j}) , \qquad (3.23)$$

where

$$G_L^s(\mathbf{r},t_1,t_2) = -\frac{1}{2\pi} [\gamma f'' + (f')^2 f \gamma^3]$$
(3.24)

and

$$G_T^s(r,t_1,t_2) = -\frac{1}{2\pi} \frac{\gamma f'}{r}$$
(3.25)

with $f' = \partial f(r, t_1, t_2) / \partial r$. We can go further if we realize that f in our theory is related to the two-time orderparameter scaling function F in the long-time limit by⁷

$$f(r,t_1,t_2) = \sin[\pi F(r,t_1,t_2)/2] . \qquad (3.26)$$

It is then easy to show that

$$G_{L}^{s}(r,t_{1},t_{2}) = -\frac{1}{4} \frac{\partial^{2}}{\partial r^{2}} F(r,t_{1},t_{2}) , \qquad (3.27)$$

$$G_T^s(\mathbf{r},t_1,t_2) = -\frac{1}{4r} \frac{\partial}{\partial r} F(\mathbf{r},t_1,t_2) . \qquad (3.28)$$

There are then a number of interesting results that we can establish. The first result is the sum rule

$$\int d\mathbf{r} \, G_{ij}^{s}(\mathbf{r}, t_{1}, t_{2}) = 0 \,. \tag{3.29}$$

Next consider, at equal times $t_1 = t_2 = t$, the physical interpretation of G_L^s and G_T^s . G_L^s is proportional to the probability of having a wall at positions \mathbf{r}_1 and \mathbf{r}_2 with the same orientation but displaced by a distance $r = |\mathbf{r}_1 - \mathbf{r}_2|$ perpendicular to the orientation of the walls. G_T^s is proportional to the probability of having a wall at positions \mathbf{r}_1 and \mathbf{r}_2 with the same orientation but displaced by a distance r parallel to the orientation of the walls. It is easy to see that the properly normalized probability distributions are

$$f_L^s(r,t) = -4rG_L^s(r,t) = r\frac{d^2}{dr^2}F(r,t)$$
(3.30)

and

$$f_T^s(\mathbf{r},t) = -\frac{d}{dr}F(\mathbf{r},t) , \qquad (3.31)$$

and which satisfy

$$\int_{0}^{\infty} dr \, f^{s}(r,t) = 1 \tag{3.32}$$

since F(0,t)=1. In the scaling regime we can introduce

$$f_L(x) = L f_L^s(r,t) = x \frac{d^2}{dx^2} F(x)$$
, (3.33)

$$f_T(x) = L f_T^s(r,t) = -\frac{d}{dx} F(x)$$
, (3.34)

which gives a set of invariant probability distributions. It is shown analytically in Ref. 6 that for small x,

$$F = 1 - \alpha x \left[1 - \frac{1 + \pi/6\mu}{4d + 2} x^2 + \cdots \right], \qquad (3.35)$$

where

$$\alpha = \sqrt{2/\pi\mu(d-1)} \tag{3.36}$$

and $\mu(d)$ is a nonlinear eigenvalue which depends on d (e.g., $\mu = 1.104$ for d = 2 and 0.5917 for d = 3). We then easily obtain that

$$f_L(x) = \frac{3\alpha(1 + \pi/6\mu)}{2d + 1} x^2 + \cdots, \qquad (3.37)$$

$$f_T(x) = \alpha \left[1 - \frac{3 + \pi/2\mu}{4d + 2} x^2 + \cdots \right].$$
 (3.38)

For large x one has

$$F(x) \sim x^{d - \pi/2\mu} e^{-x^2/2} , \qquad (3.39)$$

and therefore we find

$$f_L(x) \sim x^{d+3-\pi/2\mu} e^{-x^2/2}$$
(3.40)

while

$$f_T(\mathbf{x}) \sim \mathbf{x}^{d+1-\pi/2\mu} e^{-\mathbf{x}^2/2}$$
 (3.41)

Comparing (3.37) and (3.40) we expect $f_L(x)$ to have a peak value at a nonzero value of x indicating that independent walls are on the average separated by a distance $L(t)x_0$ where x_0 is the peak position of $f_L(x)$. On the other hand, by comparing (3.38) and (3.41) we observe f_T to be monotonically decreasing in x. The physical interpretation is that at short distances along the parallel to a wall it is very likely that one will encounter the same wall.

IV. POINT DEFECTS n = d

In the case of point defects we consider the correlations of the density $\rho(\mathbf{r},t)$ given by (1.7). One must, however, be careful to properly treat the self-interactions. Clearly, using (2.13), we have

$$\rho(\mathbf{r}_1,t)\rho(\mathbf{r}_2,t) = \sum_{\alpha} q_{\alpha}^2 \delta(\mathbf{r}_1 - \mathbf{x}_{\alpha})\delta(\mathbf{r}_2 - \mathbf{x}_{\alpha}) + \sum_{\alpha \neq \beta} q_{\alpha} q_{\beta} \delta(\mathbf{r}_1 - \mathbf{x}_{\alpha})\delta(\mathbf{r}_2 - \mathbf{x}_{\beta})$$

$$= \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{m}(1)) |\det \partial \mathbf{m}(1)| + \delta(\mathbf{m}(1)) \delta(\mathbf{m}(2)) \det \partial \mathbf{m}(1) \det \partial \mathbf{m}(2)$$

(4.1)

where in the second term we restrict $\mathbf{r}_1 \neq \mathbf{r}_2$. The correlation function can then be written in the form

$$G(\mathbf{r},t) = \delta(\mathbf{r})n_0(t) + g(\mathbf{r},t) , \qquad (4.2)$$

where

$$n_0(t) = \langle \delta(\mathbf{m}(1)) | \det \partial \mathbf{m}(1) | \rangle$$
(4.3)

is the unsigned density of defects and

$$g(\mathbf{r},t) = \langle \delta(\mathbf{m}(1)) \delta(\mathbf{m}(2)) \det \partial \mathbf{m}(1) \det \partial \mathbf{m}(2) \rangle . \qquad (4.4)$$

As it turns out, the determination of $n_0(t)$ is actually more difficult than $g(\mathbf{r}, t)$ because of the absolute value of the determinant required in the calculation. Using the integral representation

$$\operatorname{sgn}(x) = \int d\omega \frac{\sin \omega x}{\pi \omega}$$
, (4.5)

we can rewrite (4.3) in the more promising form

$$n_0(t) = -\int \frac{d\omega}{\pi\omega} \frac{\partial}{\partial\omega} \operatorname{Re} \langle \,\delta(\mathbf{m}) \exp(i\omega \,\det\partial\mathbf{m}) \,\rangle \quad (4.6)$$

Using here, and below, the representation for the determinant

$$\det \partial \mathbf{m} = \sum_{i_1 i_2 \cdots i_n} \epsilon_{i_1 i_2 \cdots i_n} \partial_{i_1} m_1 \partial_{i_2} m_2 \cdots \partial_{i_n} m_n , \qquad (4.7)$$

we can rewrite (4.6) in the form

$$n_{0}(t) = -\int \frac{d\omega}{\pi\omega} \frac{\partial}{\partial\omega} \operatorname{Re} \int \frac{d^{d}\mathbf{k}}{(2\pi)^{d}} \left\langle \exp\left[i\mathbf{k}\cdot\mathbf{m} + i\omega\sum_{i_{n}} \mathcal{Q}_{i_{n}}\partial_{i_{n}}m_{n}\right] \right\rangle, \qquad (4.8)$$

where

$$Q_{i_n} = \sum_{i_1 \cdots i_{n-1}} \epsilon_{i_1 \cdots i_{n-1} i_n} \partial_{i_1} m_1 \cdots \partial_{i_{n-1}} m_{n-1} .$$

$$(4.9)$$

We see immediately that the average over m_n is of the same form as (3.4) and one easily obtains

$$\left\langle \exp\left[i\mathbf{k}\cdot\mathbf{m}+i\omega\sum_{i_{n}}Q_{i_{n}}\partial_{i_{n}}m_{n}\right]\right\rangle = e^{-S_{0}k_{n}^{2}/2}\int\frac{d^{n}\mathbf{y}^{(1)}}{(2\pi)^{n/2}}e^{-(\mathbf{y}^{(1)})^{2}/2}\left\langle \exp\left[i\sum_{l=1}^{n-1}k_{l}m_{l}+i\omega\sum_{i_{n-1}}Q_{i_{n-1}}^{(1)}\partial_{i_{n-1}}m_{n-1}\right]\right\rangle, (4.10)$$

where

$$Q_{i_{n-1}}^{(1)} = \sum_{i_1, i_2, \cdots, i_{n-2}, i_n} \epsilon_{i_1, \cdots, i_n} \partial_{i_1} m_1 \cdots \partial_{i_{n-2}} m_{n-2} \sqrt{S_2} y_{i_n}^{(1)} .$$
(4.11)

Equation (4.11) has the same structure as (3.4). We continue this process n times to obtain

$$n_{0}(t) = -\int \frac{d\omega}{\pi\omega} \frac{\partial}{\partial\omega} \operatorname{Re} \int \frac{d^{n}\mathbf{k}}{(2\pi)^{n}} e^{-S_{0}\mathbf{k}^{2}/2} \int \prod_{i=1}^{n} \frac{d^{n}\mathbf{y}^{(i)}}{(2\pi)^{n/2}} \exp\left[-\frac{1}{2}\sum_{i=1}^{n} (\mathbf{y}^{(i)})^{2}\right] \\ \times \exp\left[i\omega(S_{2})^{n/2}\sum_{i_{1}i_{2}\cdots i_{n}} y_{i_{1}}^{(1)}y_{i_{2}}^{(2)}\cdots y_{i_{n}}^{(n)}\epsilon_{i_{1}i_{2}}\cdots i_{n}\right].$$
(4.12)

After performing the **k** integration and rescaling ω by a factor of $S_2^{n/2}$ we obtain

$$n_0(t) = \left[\frac{S_2}{S_0}\right]^{n/2} C_n , \qquad (4.13)$$

where the coefficients are given by

$$C_n = -\int \frac{d\omega}{\pi\omega} \frac{\partial}{\partial\omega} \int \prod_{i=1}^n \frac{d^n \mathbf{y}^{(i)}}{(2\pi)^n} \exp\left[-\frac{1}{2} \sum_{i=1}^n (\mathbf{y}^{(i)})^2\right] \exp\left[i\omega \sum_{i_1 i_2 \cdots i_n} y_{i_1}^{(1)} y_{i_2}^{(2)} \cdots y_{i_n}^{(n)} \epsilon_{i_1 i_2 \cdots i_n}\right].$$
(4.14)

For small n it is easy to evaluate the C_n explicitly:

$$C_1 = \frac{1}{\pi}; \quad C_2 = \frac{1}{2\pi}; \quad C_3 = \frac{1}{\pi^2}$$
 (4.15)

We turn now to the evaluation of $g(\mathbf{r}, t)$. Using (4.4) we find

$$g(\mathbf{r},t) = \sum_{\{i,j\}} \epsilon_{i_1 i_2 \cdots i_n} \epsilon_{j_1 j_2 \cdots j_n} \langle \delta(\mathbf{m}(1)) \delta(\mathbf{m}(2)) \partial_{i_1} m_1(1) \cdots \partial_{i_n} m_n(1) \partial_{j_1} m_1(2) \cdots \partial_{j_n} m_n(2) \rangle .$$

$$(4.16)$$

For an isotropic system, the average in (4.16) can be factored into a product of averages over perpendicular components and (4.16) can be reduced to the form

DEFECT-DEFECT CORRELATION IN THE DYNAMICS OF ... 5969

$$g(\mathbf{r},t) = \sum_{\{i,j\}} \epsilon_{i_1 i_2 \cdots i_n} \epsilon_{j_1 j_2 \cdots j_n} A_{i_1 j_1} A_{i_2 j_2} \cdots A_{i_n j_n}, \qquad (4.17)$$

where

$$A_{ij}(\mathbf{r},t) = \langle \,\delta(m_1(1))\delta(m_1(2))\partial_i m_1(1)\partial_j m_1(2) \,\rangle \ . \tag{4.18}$$

We notice at once that A_{ii} is precisely the quantity we evaluated in the scalar case (3.14) and we obtain immediately

$$A_{ij}(\mathbf{r},t) = A_L(\mathbf{r},t)\hat{\mathbf{r}}_i\hat{\mathbf{r}}_j + A_T(\mathbf{r},t)(\delta_{ij} - \hat{\mathbf{r}}_i\hat{\mathbf{r}}_j)$$
(4.19)

with

$$A_T = \frac{h(r,t)}{r} , \qquad (4.20)$$

$$A_L = \frac{\partial h(r,t)}{\partial r} , \qquad (4.21)$$

where as before $h(r) = -\gamma f'/2\pi$. Inserting (4.19) into (4.17) we obtain

$$\mathbf{g}(\mathbf{r},t) = \sum_{\{i,j\}} \boldsymbol{\epsilon}_{i_1 \cdots i_n} \boldsymbol{\epsilon}_{j_1 \cdots j_n} \left[\frac{h}{r} \delta_{i_1 j_1} + \left(\frac{\partial h}{\partial r} - \frac{h}{r} \right) \mathbf{\hat{r}}_{i_1} \mathbf{\hat{r}}_{j_1} \right] \cdots \left[\frac{h}{r} \delta_{i_n j_n} + \left(\frac{\partial h}{\partial r} - \frac{h}{r} \right) \mathbf{\hat{r}}_{i_n} \mathbf{\hat{r}}_{j_n} \right].$$
(4.22)

Expanding the product in (4.22), terms can be grouped such that

$$g(\mathbf{r},t) = n! \left[\frac{h}{r}\right]^{n} + \left[\frac{h}{r}\right]^{n-1} \left[\frac{\partial h}{\partial r} - \frac{h}{r}\right]_{\{i\},j} \boldsymbol{\epsilon}_{i_{1}} \cdots i_{n} \mathbf{\hat{r}}_{j} (\boldsymbol{\epsilon}_{j_{i_{2}}} \cdots i_{n} \mathbf{\hat{r}}_{i_{1}} + \boldsymbol{\epsilon}_{i_{1}j} \cdots i_{n} \mathbf{\hat{r}}_{i_{2}} + \cdots + \boldsymbol{\epsilon}_{i_{1}} \cdots i_{n} \mathbf{\hat{r}}_{i_{n}}).$$
(4.23)

All higher-order terms vanish because each term will involve a product $\sum_{i_{\alpha}i_{\beta}} \hat{\mathbf{r}}_{i_{\alpha}} \hat{\mathbf{r}}_{i_{\beta}} \boldsymbol{\epsilon} \cdots \boldsymbol{i}_{\alpha} \cdots \boldsymbol{i}_{\beta} \cdots$ which is odd under the permutation of the two specified indices. After straightforward algebra, (4.23) can be written as

$$g(\mathbf{r},t) = n! \left[\frac{h}{r}\right]^{n-1} \frac{\partial h}{\partial r} . \qquad (4.24)$$

Now charge neutrality requires

$$\int G(\mathbf{r},t)d\mathbf{r}=0 \tag{4.25}$$

or, using (1.6),

$$n_0(t) = -\int g(\mathbf{r}, t) d\mathbf{r} . \qquad (4.26)$$

The integral in (4.26) can be readily evaluated using (4.24) to give

$$n_0(t) = \frac{n! \pi^{n/2}}{(2\pi)^n \Gamma(1+n/2)} \lim_{r \to 0} (-\gamma f')^n .$$
 (4.27)

Assuming that f(r, t) is analytic in r up to $O(r^2)$:

$$f = 1 - (S_2 / 2S_0)r^2 + \cdots$$
 (4.28)

we easily obtain

$$n_0(t) = \frac{n! [S_2/S_0]^{n/2}}{2^n \pi^{n/2} \Gamma(1+n/2)} .$$
(4.29)

Comparing (4.29) with (4.13) we obtain

$$C_n = \frac{n!}{2^n \pi^{n/2} \Gamma(1+n/2)} . \tag{4.30}$$

For n = 1, 2, and 3 this result agrees with our direct calculation (4.15) and appears to provide a general evaluation of the integral given by (4.14).

We are now in a position to analyze our general expression for $g(\mathbf{r},t)$ which we write in terms of scaling variables $\mathbf{x} = \mathbf{r}/L(t)$ in the form

$$g(\mathbf{r},t) = \frac{1}{L^{2n}(t)} \tilde{g}(\mathbf{x})$$
(4.31)

and

$$\widetilde{g}(\mathbf{x}) = \frac{(n-1)!}{x^{n-1}} \frac{d}{dx} \widetilde{h}^{n}(x) , \qquad (4.32)$$

where $\tilde{h}(x) = -\gamma f'(x)/2\pi$.

We can treat $\tilde{g}_n(x)$ analytically in the limit of small and large x. Consider first the small-x behavior. We have from Ref. 11 the expansion

$$f(x) = 1 - \frac{\alpha}{2} x^2 (1 + \Delta(x))$$
, (4.33)

where, for small x, Δ is given to leading order by

$$\Delta(x) \sim \begin{cases} -\frac{1}{\ln x} & \text{for } n = 2 \\ x & \text{for } n = 3 \\ -x^2 \ln x & \text{for } n = 4 \\ x^2 & \text{for } n > 4 \end{cases}$$
(4.34)

From (4.33) it is easy to extract the leading behavior for \tilde{g} at small x:

<u>46</u>

$$\widetilde{g}(x) \sim \frac{\Delta'(x)}{x^{n-1}} \sim \begin{cases} \frac{1}{x^2 \ln^2 x} & \text{for } n = 2\\ \frac{1}{x^2} & \text{for } n = 3\\ -\frac{\ln x}{x^2} & \text{for } n = 4\\ \frac{1}{x^{n-2}} & \text{for } n > 4 \end{cases}$$
(4.35)

In the large-x limit, where f falls off exponentially,

$$f(x) \sim \exp(-x^2/2)$$
 (4.36)

we conclude that

$$\tilde{g}(x) \sim -x^2 \exp(-nx^2/2)$$
 (4.37)

which decays rapidly to zero.

 $\tilde{g}(x)$ can be determined from (4.32) for all x by using our numerical determination for f(x) given in Ref. 11. The result for n = d = 2 is shown in Fig. 1. Also shown are the numerical results of Mondello *et al.*¹⁸ for a complex order parameter in 2D. In the large-distance regime, our result agrees qualitatively with the simulation. However, a disturbing discrepancy is observed at short distances. While the numerical simulation gives $g(x) \rightarrow 0$ as $x \rightarrow 0$, our calculation suggests a positive divergence. This divergence comes from the higher-order singular terms $\Delta(x)$ in the expansion of f(x). For comparison, we also plot $\tilde{g}(x)$ evaluated using the form f(x) $= \exp(-x^2/2)$ used in the Ohta-Jasnow-Kawasaki (OJK) approach.³

For n = d = 2 one has the special case of a lower critical dimensionality. Thus the analysis for nonzero temperature requires treating bound vortex pairs and spin waves and algebraic decay of the order-parameter correlation function. It seems likely that our analysis here must be modified for n = d = 2 to include the self-consistent disordering aspects of spin waves even for



FIG. 1. Defect correlation functions. Solid squares are data from 2D numerical simulations of a complex order parameter in Ref. 18. Solid curve is calculated from the theory in this paper using (4.32) for n = d = 2. Dashed curve is from the OJK-type approach. Abscissa for the curves is scaled so as to give a best fit to the data at large x. Dotted line is the prediction from (4.32) for n = d = 3.

quenches to zero temperature. We intend to discuss this special case elsewhere.

V. STRING DEFECTS, n = d - 1

This case n = d - 1 where the defects are strings or vortex lines is relevant to the interesting examples of a 3D neutral superfluid (n = 2, d = 3), as well as the wellknown 2D scalar Ising system. The string density operator is now defined by (2.17). Note that the δ function is defined in the *n*-dimensional order parameter space while the antisymmetric tensor is defined over permutations $\{ii_1i_2\cdots i_n\}$ in the *d*-dimensional physical space. The string-string correlation function now reads

$$G_{ij}(\mathbf{r},t) = \langle \rho_i(1)\rho_j(2) \rangle$$

= $\epsilon_{ii_1i_2\cdots i_n}\epsilon_{jj_1j_2\cdots j_n} \langle \delta(\mathbf{m}(1))\delta(\mathbf{m}(2))\partial_{i_1}m_1(1)\cdots \partial_{i_n}m_n(1)\partial_{j_1}m_1(2)\cdots \partial_{j_n}m_n(2) \rangle$ (5.1)

which, as before, can be cast into the form

$$G_{ij}(\mathbf{r},t) = \epsilon_{ii_1} \cdots i_n \epsilon_{jj_1} \cdots j_n A_{i_1j_1} A_{i_2j_2} \cdots A_{i_nj_n} , \qquad (5.2)$$

where A_{ij} is again given by (4.19). Following an analysis similar to the n = d case we obtain

$$G_{ij}(\mathbf{r},t) = G_T(\mathbf{r},t)(\delta_{ij} - \hat{\mathbf{r}}_i \hat{\mathbf{r}}_j) + G_L(\mathbf{r},t)\hat{\mathbf{r}}_i \hat{\mathbf{r}}_j , \qquad (5.3)$$

where $G_L(\mathbf{r},t) = n!(h/r)^n$ and the transverse part has the same form as $g(\mathbf{r},t)$ for n = d. In this form it is easy to show that "charge" conservation is satisfied:

$$\int G_{ij}(\mathbf{r},t) d^d \mathbf{r} = 0 . \qquad (5.4)$$

In terms of the scaled variable, the large-x behavior of $G_L(\mathbf{x})$ is easy to extract:

$$G_L(\mathbf{x}) \sim \exp(-nx^2/2)$$
 (5.5)

At short distances, since $h(x \rightarrow 0) = \text{const.}$, we have

$$G_L(\mathbf{x}) \sim x^{-n} \text{ for } \mathbf{x} \to 0$$
 (5.6)

Again numerical results are available for this system. Mondello *et al.*¹⁹ measured a *scalar* string-string correlation function $\Gamma_{ss}(x)$. Unfortunately this quantity is not simply related to the correlation function G_{ij} calculated here. We cannot therefore attempt a fit to the numerical results. However, it is easy to realize that the shortdistance behavior of Γ_{ss} is governed by that of the longitudinal part of G_{ij} . Thus we have

$$\Gamma_{\rm ss}(x) \sim x^{-2} , \qquad (5.7)$$

which is precisely what is found in numerical simulations.

To summarize, we have calculated, starting from some quite reasonable physical assumptions, various defectdefect correlation functions. These correlations satisfy scaling in the late stages of phase ordering. The functional form of the resulting functions depend more sensitively, particularly at short distances, on the structure of the theory than the usual order-parameter correlation function.

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