Defect coarsening and spin waves in the nonlinear σ model

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We propose a phenomenological equation of motion for the nonlinear σ model undergoing defect coarsening at low temperatures, in which the thermal fluctuation degrees of freedom (spin waves) are explicitly separated from the defect degrees of freedom. The Gaussian closure approximation is used to find the zero temperature order parameter correlation function. The main result of this paper is the calculation of the spin wave correlation function, which is the $O(T)$ correction to the order parameter correlation function. The spin wave correlation function shows the scaling behavior predicted by Bray [Phys. Rev. Lett. **62**, 2841 (1989)] for $N > 2$, and is exact in the $t \to \infty$ and $N \to \infty$ limits. Our results for the XY model in two dimensions clarify the nature of coarsening observed at the lower critical dimension.

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I. INTRODUCTION

There has been a great deal of progress recently in the theory of defect coarsening at first order phase transitions [1–5]. These systems typically evolve into a scaling regime, in which all statistical properties depend on time only through a single, time-dependent length scale $L(t)$. Because the scaling regime is believed to arise from a zero temperature fixed point [6], the effects of temperature on the coarsening dynamics have been largely overlooked. One important effect of temperature is the excitation of spin waves in the regions between defects. These are the precursors to the well-known Nambu-Goldstone modes in a completely ordered system [7, 8]. The spin waves renormalize the interaction between defects, and they are interesting in their own right.

In this paper we consider the coarsening of a nonconserved, N-component order parameter $\vec{\psi}$ in d dimensions, as modeled by the nonlinear σ (NLS) model. We propose a separation of the order parameter into "fast" modes $\vec{v}$ due to thermal fluctuations and "slow" modes $\vec{\sigma}$ representing the underlying defect dynamics. This separation is only approximate, but it has a strong phenomenological motivation. It is worth developing because it allows us to calculate the order parameter correlation function at nonzero temperature. Our results illuminate the role of thermal fluctuations in coarsening systems and reproduce known exact results.

We calculate the correlation function of the ordering modes $\langle \sigma_i | \sigma_j \rangle = C_{\sigma\sigma}(r,t)\delta_{ij}$ using the standard Gaussian closure approximation [2–5]. [We will consistently use the shorthand $\langle A|B\rangle$ for $\langle A(\mathbf{r}',t)B(\mathbf{r}'+\mathbf{r},t)\rangle$.] This calculation is nearly identical to those made previously by Liu and Mazenko [4] and Bray [5] for the time-dependent Ginzburg-Landau (TDGL) model. As expected, we find a scaling solution $C_{\sigma\sigma}(r,t) = G(r/L)$ with $L \sim t^{1/2}$. The function G depends upon N and d and is quantitatively similar to that calculated for the TDGL model.

We go on to make a Gaussian assumption for the thermal fluctuations $\vec{v}$ and to calculate the correlation function $\langle v_i | v_j \rangle = C_{vv}(r,t)\delta_{ij}$. This is the primary result of our paper. The calculation presented is analagous to the usual Gaussian approximation for fluctuations around the ferromagnetically ordered state [8]. For $N > 2$ we find that C_{vv} has the scaling form $C_{vv} = TL^{2-d}F(r/L)$ first predicted by Bray [6]. The function F depends upon N and d, and is *exact* in the $N \to \infty$ and $t \to \infty$ limits. For $N = 2$, we find that $C_{vv} = Tl^{2-d}F(r/l)$ where $l = L/[\ln(L/a)]^{1/2}$.

Coarsening at the lower critical dimension $d = d_c = 2$ requires special consideration. Coarsening is frequently described as a process that takes place at a first-order symmetry breaking phase transition, but the NLS model in $d_c = 2$ is known to have no broken symmetry phase at $T > 0$ [9]. Nevertheless, Yurke *et al.* [10] performed simulations of the XY model (N=2) in two dimensions and observed qualitatively normal coarsening at a range of temperatures below the Kosterlitz-Thouless transition temperature. We will resolve this apparent paradox in Sec. VI.

This paper is organized as follows. In Sec. II, we review the NLS model as applied to defect coarsening. In Sec. III, we develop the separation between $\vec{\sigma}$ and $\vec{v}$. In Sec. IV, we briefly review the methods developed for coarsening at zero temperature and apply them to $\vec{\sigma}$. In Sec. V, we develop the Gaussian approximation for $\vec{v}$ and calculate C_{vv}. In Sec. VI, we discuss the peculiarities of coarsening at $d_c = 2$.

II. NLS MODEL

The NLS model has an N-component order parameter $\vec{\psi}(\mathbf{r},t)$ with fixed length $\psi^2 = \psi_0^2$. (We choose $\psi_0 = 1$ without loss of generality.) The NLS equation of motion at temperature T is

$$\frac{\partial \psi_i}{\partial t} = \Gamma(\nabla^2 \psi_i - \left(\vec{\psi} \cdot \nabla^2 \vec{\psi}\right) \psi_i) + \eta_i - \left(\vec{\psi} \cdot \vec{\eta}\right) \psi_i, \quad (2.1)$$

where Γ is a kinetic coefficient, and $\vec{\eta}$ is a Gaussian white noise with

$$\langle \eta_i(\mathbf{r},t)\eta_j(\mathbf{r}',t')\rangle = 2T\Gamma\delta_{ij}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \ . \quad (2.2)$$

It is important to remember that $\vec{\psi}$ is implicitly a coarse-grained quantity with a lower length scale a (in practice, the lattice spacing).

Our initial condition has mean zero and no correlations on scales greater than a, representing an instantaneous quench from a high temperature, disordered phase. One realization of this is $\langle\psi_i|\psi_j\rangle_{t=0} = \frac{1}{N}\delta_{ij}\exp(-r/a)$. Simulations of the NLS model at $T < T_c$ starting from a disordered initial condition in $d \geq N$ show the rapid formation of a dense collection of defects with dimension $d - N$ [11]. Due to the local conservation of topological charge, point defects are stable and defects of higher dimension are metastable [12]. The subsequent evolution of the order parameter is thus dominated by the motion and annihilation of defects.

It has now been well established by experiments and simulations [5, 11, 13, 14] that systems of this type exhibit scaling. There is a regime where all statistical properties depend on time only through a single, time-dependent length scale L. The two quantities of greatest interest are the growth law $L(t)$ and the order parameter correlation function $\langle\psi_i|\psi_j\rangle = C_{\psi\psi}\delta_{ij}$. It is now known that $L \sim t^{1/2}$ for a nonconserved order parameter in $d > 2$ and $d \geq N$ and that the correlation function satisfies the scaling relation $C_{\psi\psi}(r,t) = \psi_0^2 G(r/L)$. There is extensive support for this result from numerical studies [11], from heuristic arguments [15], and from the approximate theories to be discussed below. It is believed that $G(x)$ depends upon N and d, but is otherwise universal. It should be mentioned that there are few systematic studies of the effects of temperature on the coarsening of a vector order parameter. Nevertheless, by analogy with other coarsening systems it is believed that scaling results from a zero temperature fixed point, and that temperature is an irrelevant variable at that fixed point [6]. This implies that $G(x)$ is independent of temperature, up to appropriate redefinitions of ψ_0^2 and $L(t)$. In the theory developed below, we find that $C_{\psi\psi}(r,t) = [1 + O(T)]G(r/L) + O(TL^{2-d})$ for $d > 2$ and $d \geq N$, in agreement with this expectation.

There are two exactly solvable limits for the NLS model at nonzero temperature $0 < T \ll T_c$. At $t = \infty$, the system is ferromagnetically ordered and the noise excites Nambu-Goldstone modes $\vec{u}$ with two-point correlation function $C_{uu}(k) = T/k^2$ [8]. At $N = \infty$, Mazenko and Zannetti [16] calculated the order parameter correlation function in the scaling regime

$$C_{\psi\psi}(k,t) = L^d \frac{(1 - c_d T)(2\pi)^{d/2}}{N} e^{-K^2/2} + TL^2 \frac{1 - e^{-K^2/2}}{K^2}, \tag{2.3}$$

where c_d is a constant that depends on d, $K = kL$ is the scaled wave number, and $L = 2(\Gamma t)^{1/2}$. Note that this reproduces the correct $t \to \infty$ limit.

III. SEPARATION OF THE DEGREES OF FREEDOM

We will use Eq. (2.3) to motivate the calculation of this section. The correlation function $C_{\psi\psi}$ is written as the sum of two terms. The first term is the standard $T = 0$ result, up to a temperature-dependent constant. It is due to the presence of large, ordered regions of size $\sim L$, and it reproduces the Bragg peak as $t \to \infty$. The second term is $O(T)$ and is due to transverse thermal fluctuations about the partly ordered state. We are thus tempted to write $\vec{\psi} = \vec{\sigma} + \vec{v}$, where $\vec{\sigma}$ orders like $\vec{\psi}$ at $T = 0$ (and includes the defects) and $\vec{v}$ represents the transverse fluctuations. Assuming $C_{\sigma v} = 0$, we then have $C_{\psi\psi} = C_{\sigma\sigma} + C_{vv}$. We expect $v^2 \sim \eta^2 \sim T$ by analogy with the ordered case.

To motivate this separation another way, consider the NLS model at $T = 0$. We define the time scale τ_σ as an estimate of the time it takes $\vec{\psi}$ to change by order unity. In the scaling regime, changes in $\vec{\psi}$ are predominantly due to the motion of nearby defects. Using an argument due to Bray and Rutenberg [15], we can approximate $\partial\vec{\psi}(\mathbf{r})/\partial t \sim \mathbf{v}\cdot\nabla\vec{\phi}(\mathbf{r}-\mathbf{r}')$, where $\mathbf{v}$ is the velocity of the nearest defect, located at $\mathbf{r}'$, and $\vec{\phi}(\mathbf{R})$ is the field of an isolated defect (unique up to global rotations and reflections). In the scaling regime $v \sim L/t \sim 1/L$ and $\nabla\vec{\phi} \sim 1/R$, where R is the distance to the nearest defect. We thus have that $\tau_\sigma \sim LR$. The important thing to notice is that $\tau_\sigma|_{\min} \sim La$ diverges with L. In this sense, coarsening is related to the presence of asymptotically slow modes in the system.

The belief that coarsening is governed by a zero temperature fixed point implies that the slow modes are still present in the system at finite temperature. We label the slow modes $\vec{\sigma}$. The noise gives rise to transverse fluctuations in $\vec{\psi}$, which we will treat as a small perturbation around $\vec{\sigma}$. We label the fluctuations $\vec{v}$. It should be clear that the typical length and time scales in $\vec{v}$ are microscopic, so that the separation between $\vec{\sigma}$ and $\vec{v}$ is roughly equivalent to a separation of time scales in the order parameter. This separation cannot be exact due to the fact that $\vec{v}$ does contain some slow modes, but we will see that it is an excellent first approximation.

We write $\vec{\psi} = \vec{\sigma} + \vec{v} + O(v^2)$, where the transverse fluctuations $\vec{v}$ satsfy $v \ll \sigma$ and $\vec{v}\cdot\vec{\sigma} = 0$. To first order in v, $\sigma^2 = \psi^2 = 1$. The issue of corrections to second order in v will be addressed in Sec. VI. To derive the equations of motion for $\vec{\sigma}$ and $\vec{v}$, we substitute $\psi_i = \sigma_i + v_i$ into the NLS equation of motion and expand to first order in $\vec{v}$ and $\vec{\eta}$. Since most $\tau_v \ll \tau_\sigma$, we can separate the equations by order to get

$$\frac{\partial\sigma_i}{\partial t} = \Gamma(\nabla^2\sigma_i + (\nabla\sigma)^2\sigma_i), \tag{3.1}$$

$$\frac{\partial v_i}{\partial t} = \Gamma(\nabla^2 v_i + 2(\nabla_k\sigma_j\nabla_k v_j)\sigma_i + (\nabla\sigma)^2 v_i) + \eta_i - (\sigma\cdot\eta)\sigma_i \tag{3.2}$$

where repeated indices are to be summed over and where we have used $\sigma^2 = 1$ and $\vec{\sigma}\cdot\vec{v} = 0$. Equation (3.1) is just the NLS equation of motion at zero temperature.

Equation (3.2) is not a self-consistent equation of motion for $\vec{v}$. The term $(\nabla\sigma)^2 v_i$ destabilizes fluctuations with wavelength $\lambda_v \gtrsim R$, and can cause v^2 to increase to order unity. A detailed calculation of C_{vv} proceeding from Eq. (3.2) yields nonphysical results. We therefore drop the $(\nabla\sigma)^2 v_i$ term *ad hoc* to get

$$\frac{\partial v_i}{\partial t} = \Gamma(\nabla^2 v_i + 2(\nabla_k \sigma_j \nabla_k v_j)\sigma_i) + \eta_i - (\vec{\sigma}\cdot\vec{\eta})\sigma_i. \tag{3.3}$$

This is the evolution equation we use for $\vec{v}$.

Equations (3.1) and (3.3) retain the essential physics of the problem:

(i) The slow modes $\vec{\sigma}$ order like $\vec{\psi}$ at $T = 0$.

(ii) Equation (3.3) preserves the constraint $\vec{\sigma}\cdot\vec{v} = 0$. It can be rewritten as $\{\dot{v}_i = \Gamma\nabla^2 v_i + \eta_i\}_{\perp\sigma}$ where $\{a_i\}_{\perp\sigma} = a_i - (\vec{\sigma}\cdot\vec{a})\sigma_i$ is a projection operator.

(iii) We can check that all $\vec{v}$ modes are stable. We have

$$\frac{\partial v^2}{\partial t} = \Gamma(\nabla^2 v^2 - 2(\nabla v)^2) + \vec{v}\cdot\vec{\eta}. \tag{3.4}$$

In the absence of noise, we see that v^2 is bounded and tends to zero. We thus expect that $v \sim \eta \sim O(\sqrt{T})$ is well behaved for all times.

(iv) If $\vec{\sigma}$ is ferromagnetically ordered, then $\dot{\sigma}_i = 0$ and Eq. (3.3) reduces to the usual equation of motion for small transverse fluctuations around the ordered state.

Furthermore, the equations are invariant under $\vec{\sigma} \to -\vec{\sigma}$ and also under $\vec{v} \to -\vec{v}$. The immediate consequence of this is that $C_{v\sigma} = 0$, and similarly for all odd correlation functions.

It is instructive to consider a single spin wave with wavevector $\mathbf{k}$, phase ϕ, and polarization $\hat{e}$: $\vec{v}_{\mathbf{k}} = v_{\mathbf{k}}\hat{e}\cos(\mathbf{k}\cdot\mathbf{r} + \phi)$. The condition $\vec{v}\cdot\vec{\sigma} = 0$ becomes the boundary condition $\vec{v}|_{\mathcal{S}_{\hat{e}}} = 0$, where $\mathcal{S}_{\hat{e}}$ is the $d - N + 1$ dimensional surface on which $\hat{e}\cdot\vec{\sigma} = \pm 1$. The boundary surfaces $\mathcal{S}$ will only intersect at defects. Indeed, since $\vec{\psi}$ attains all possible orientations in the neighborhood of a defect, each defect is threaded by all surfaces $\mathcal{S}$. The typical curvature and the typical separation of the surfaces can thus be characterized by $L(t)$.

In $N = 2$, the $\mathcal{S}$ have dimension $d - 1$. Each $\mathcal{S}_{\hat{e}}$ therefore partitions the space into separate regions of size $\sim L$ and we expect that all spin waves with wave number $k \lesssim 1/L$ will be suppressed. In $N > 2$ the $\mathcal{S}$ do not partition the space, but we still expect their presence to inhibit long-wavelength modes. (Remember that the surfaces will move around as $\vec{\sigma}$ evolves.) It is this condition which introduces the length L into C_{vv} and which cuts off the long wavelength divergence of the Nambu-Goldstone modes [consider the $N = \infty$ limit, Eq. (2.3)]. Note that the boundary conditions on $\vec{v}$ are qualitatively different for $N = 2$. This is the first indication that the case $N = 2$ is special.

One technical point is that most of the previous theoretical work has been done on the time-dependent Ginzburg-Landau model. In the TDGL model the magnitude of the order parameter is not constrained, so one needs to include the effects of longitudinal fluctuations in $\vec{\psi}$. We are working with the NLS model to avoid this complication. Preliminary calculations on the TDGL model indicate that the fluctuating degrees of freedom can still be separated and that the equation of motion for transverse fluctuations is unchanged to leading order.

IV. $C_{\sigma\sigma}$

All the results presented in this section for the NLS model are analagous to those derived in Liu and Mazenko [4] for the TDGL model. The reader is referred there for a detailed treatment.

There already exists an approximate theory for coarsening at $T = 0$ [3–5], which we can apply directly to the calculation of $C_{\sigma\sigma}$. The theory is sometimes referred to as a Gaussian closure scheme, since it relies upon a mapping from the $\vec{\sigma}$ field, which is clearly not Gaussian due to the constraint $\sigma^2 = 1$, to a new field $\vec{m}$, which can be successfully approximated as a Gaussian field. The mapping is chosen so that the zeros of $\vec{\sigma}$ coincide with the zeros of $\vec{m}$ and so that σ^2 approaches its ordered value as m gets large. The obvious choice for the NLS model is $\vec{\sigma} \equiv \hat{m} = \vec{m}/m$, with the implicit cutoff $\sigma = 0$ when $m < a$. This relation lets us write $\vec{\sigma}$ correlation functions as $\vec{m}$ correlation functions and thereby, since $\vec{m}$ is Gaussian, in terms of the two-point correlation function $\langle m_i | m_j\rangle = C_{mm}(r,t)\delta_{ij}$. We can calculate the $\vec{\sigma}$ correlation function $\langle \hat{m}_i | \hat{m}_j\rangle = C_{\sigma\sigma}(r,t)\delta_{ij}$. The result is

$$C_{\sigma\sigma} = \frac{f}{2\pi}B^2\left(\frac{1}{2},\frac{N+1}{2}\right)F\left(\frac{1}{2},\frac{1}{2};\frac{N+2}{2};f^2\right), \tag{4.1}$$

where $f = C_{mm}(r,t)/C_{mm}(0,t)$, F is the hypergeometric function, and $B(x,y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$ is the beta function.

As described in detail by Liu and Mazenko [4] and Bray [5], the order parameter evolution equation (3.1) can be used to uniquely determine C_{mm} [and therefore $C_{\sigma\sigma}$ via Eq. (4.1)]. We enforce

$$\left\langle \frac{\partial\sigma_i}{\partial t} - \Gamma(\nabla^2\sigma_i + (\nabla\sigma)^2\sigma_i)\middle|\sigma_i\right\rangle_m = 0 \tag{4.2}$$

(note that i is not to be summed over here or below). After calculating the $\vec{m}$ averages we find a differential equation to be satisfied by $f(r,t)$

$$\frac{\partial f}{\partial t} = \nabla^2 f + \frac{f}{S_0} + \frac{2}{3}\frac{\partial^2 C_{\sigma\sigma}/\partial f^2}{\partial C_{\sigma\sigma}/\partial f}(\nabla f)^2, \tag{4.3}$$

where $S_0(t) = C_{mm}(0,t)$. The derivatives of $C_{\sigma\sigma}$ with respect to f can be calculated from Eq. (4.1). Equation (4.3) supports a scaling solution with $f(r,t) = f(r/L)$, $S_0 \sim L^2$, and $L \sim t^{1/2}$. Since f scales, so does $C_{\sigma\sigma}$, and we can write $C_{\sigma\sigma}(r,t) = G(r/L)$.

Rewriting Eq. (4.3) in terms of the scaled variable $x = r/L$ yields an ordinary differential equation for $f(x)$

$$-xf' = \nabla^2 f + \frac{\pi}{2\mu}f + \frac{2}{3}\frac{\partial^2 G/\partial f^2}{\partial G/\partial f}(f')^2, \tag{4.4}$$

where we have chosen $L = 2(\Gamma t)^{1/2}$, and where a prime indicates a derivative with respect to x. The calculation of f requires the solution of a nonlinear eigenvalue problem. The quantity $\mu = \pi S_0/2L^2$ is the eigenvalue to be determined [17].

Equation (4.4) has the general large x solution $f = Ax^{-d+\pi/2\mu}e^{-x^2/2} + Bx^{-\pi/2\mu}$, where A and B are undetermined constants. The physical solution is expected to

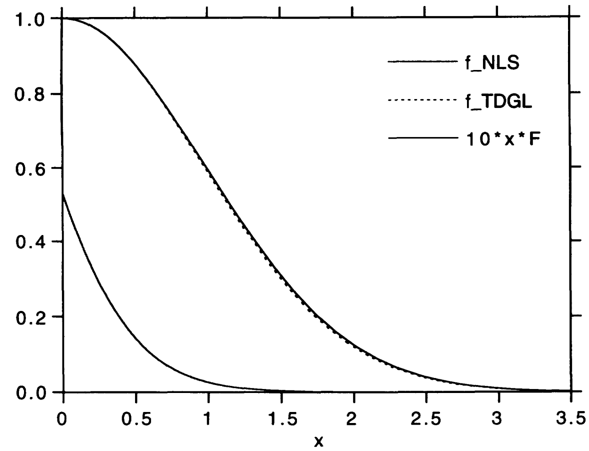

FIG. 1. The functions $f_{\rm NLS}(x)$, $f_{\rm TDGL}(x)$, and $10xF(x)$ for $N = d = 3$ corresponding to the eigenvalues $\mu_{\rm NLS} = 0.5440$, $\mu_{\rm TDGL} = 0.5558$, and $\nu = -0.1173$, respectively.

decay exponentially, and to therefore have $B = 0$. It is straightforward to determine that the small x behavior of f is $f = 1 - \alpha x^2$ with $\alpha = \pi/(4\mu d)$. The eigenvalue μ is thus uniquely determined by requiring that the short distance behavior match onto the long distance solution with $B = 0$. Since Eq. (4.4) is nonlinear, the problem must be solved numerically.

It should be noted that the differential equation to be satisfied by $f(x)$ is different for the NLS and TDGL models, but that the resulting changes in f and μ are small. The equation for $f_{\rm TDGL}$ analogous to (4.4) differs only by the replacement of the factor 2/3 by 1. This replacement leaves the leading short and long distance behaviors of f unchanged. To check that the resulting differences are quantitatively small, we calculated μ and f for both models for $N = d = 3$. We find $\mu_{\rm NLS}(3,3) = 0.5440$ and $\mu_{\rm TDGL}(3,3) = 0.5558$, a 2% difference. Figure 1 shows the corresponding $f_{\rm NLS}$ and $f_{\rm TDGL}$. They are nearly indistinguishable, having a maximum absolute difference of about 0.01 and a maximum relative difference in the exponentially decaying tail of about 5%. Since the altered term only enters the small distance expansion at order x^N, we expect the relative difference to decrease with increasing N. Indeed, it is easy to check that $f_{\rm NLS}$ and $f_{\rm TDGL}$ both reproduce the correct limit as $N \to \infty$.

V. C_{vv}

A. The Gaussian approximation for $\vec{v}$

Now we turn our attention to the calculation of C_{vv}. In the spirit of the preceding section, we will introduce a second Gaussian approximation. We relate the field $\vec{v}$ to a new field $\vec{g}$, which is postulated to be Gaussian. Starting from the equation of motion (3.3), we derive a differential equation to be satisfied by C_{vv}. We find that C_{vv} has a scaling form, whose calculation requires the numerical solution of an eigenvalue problem.

The field $\vec{v}$ is poorly approximated by a Gaussian field, since a Gaussian field will not satisfy the orthogonality constraint $\vec{\sigma} \cdot \vec{v} = 0$. We here adopt the next simplest approach, which is to assume that $\vec{v}$ can be written $v_i = g_i - (\vec{\sigma} \cdot \vec{g})\sigma_i$, where $\vec{g}$ is a Gaussian field. This definition identically satisfies the orthogonality condition, and it reduces to the familiar Gaussian approximation for transverse fluctuations when $\vec{\sigma}$ is ferromagnetically ordered [8]. We thus have two N-component Gaussian fields, $\vec{m}$ and $\vec{g}$, and two functional relations $\vec{\sigma}[\vec{m}]$ and $\vec{v}[\vec{m}, \vec{g}]$. We know C_{mm}, as discussed in the previous section. We need to calculate $\langle g_i | m_j \rangle = C_{gm}(r,t)\delta_{ij}$ and $\langle g_i | g_j \rangle = C_{gg}(r,t)\delta_{ij}$ where the brackets now indicate averages over $\vec{m}$ and $\vec{g}$.

As discussed in Sec. III, $C_{v\sigma} = 0$, due to the symmetry of the equations of motion. We can easily show that this requires $C_{gm}(r,t) = a_0 f(r,t)$, with a_0 undetermined and $f = C_{mm}/S_0$ defined previously. This choice ensures that all correlation functions odd in v are zero.

To derive the differential equation to be satisfied by C_{vv}, we recall Eq. (3.3) and demand

$$\langle -\dot{v}_i + \Gamma(\nabla^2 v_i + 2(\nabla_k \sigma_j \nabla_k v_j)\sigma_i) + \eta_i - (\vec{\sigma} \cdot \vec{\eta})\sigma_i | v_i \rangle_{m,g,\eta} = 0. \quad (5.1)$$

The terms involving the noise are readily shown to be $\langle \eta_i - (\sigma \cdot \eta)\sigma_i | v_i \rangle = (1 - 1/N)T\Gamma\delta(\mathbf{r})$. Equation (5.1) then simplifies to

$$\frac{1}{2}\frac{\partial C_{vv}}{\partial t} = \Gamma(\nabla^2 C_{vv} + 2\langle(\nabla_k \sigma_j \nabla_k v_j)\,\sigma_i | v_i \rangle) + \left(1 - \frac{1}{N}\right) T\Gamma\delta(\mathbf{r}) \ . \quad (5.2)$$

We can already see the nature of the scaling solution for C_{vv} by counting powers in Eq. (5.2). Comparing left and right hand sides, we have $t \sim L^2$. Comparing the noise term with the others, we have $L^{-2}C_{vv} \sim T\delta(\mathbf{r}) \sim TL^{-d}$. We thus expect $C_{vv}(r,t) = TL^{2-d}F(r/L)$, with Fourier transform $C_{vv}(k,t) = TL^2F(kL)$. We will see that this argument is correct for $N > 2$. For the XY model, $N = 2$, this argument fails because the term $\langle(\nabla_k \sigma_j \nabla_k v_j)\,\sigma_i | v_i \rangle \sim L^{-2}\ln(L/a)$. We therefore restrict our attention to $N > 2$ in this section.

The expression for $\langle(\nabla_k \sigma_j \nabla_k v_j)\,\sigma_i | v_i \rangle$ in terms of C_{mm} and C_{gg} is not very transparent:

$$\langle(\nabla_k \sigma_j \nabla_k v_j)\,\sigma_i | v_i \rangle = \frac{1}{NS_0}\mathcal{B}_1 \tilde{C}_{gg} + \frac{1}{N}\mathcal{B}_2 \nabla f \cdot \nabla \tilde{C}_{gg} + \frac{1}{N^2}\mathcal{B}_3 (\nabla f)^2 \tilde{C}_{gg}, \quad (5.3)$$

$$\mathcal{B}_1 = \frac{N-1}{N}\left(f^2 - \frac{N-1}{N-2} - \frac{N\gamma^2}{2}\mathcal{C}_2\right), \quad (5.4)$$

$$\mathcal{B}_2 = -f + \frac{N\gamma^2}{2f}\mathcal{C}_2, \quad (5.5)$$

$$\mathcal{B}_3 = 2f^2 + \frac{\gamma^4}{4}\left[\frac{N^3}{2f^2}\mathcal{C}_4 + N^2\left(\frac{1}{2f^2} - 2\right)\mathcal{C}_3 + 2N\mathcal{C}_2 + \frac{2}{(N-2)\gamma^2}\right], \quad (5.6)$$

$$\mathcal{C}_2 = \langle\sigma_j\sigma_k|\sigma_j\sigma_k\rangle - f^2 - \frac{1}{N}\frac{1-2f^2}{\gamma^2}, \quad (5.7)$$

$$\mathcal{C}_3 = \mathcal{C}_2 - \frac{1}{N^2}\frac{2f^2}{\gamma^2}(3-4f^2), \quad (5.8)$$

$$\mathcal{C}_4 = \mathcal{C}_3 + \frac{1}{N^3}\frac{4f^2}{\gamma^2}(3-14f^2+12f^4), \quad (5.9)$$

where $\tilde{C}_{gg} = C_{gg} - a_0^2 f/S_0$ and $\gamma^2 = 1/(1-f^2)$. Note that $\mathcal{B}_1$ and $\mathcal{B}_3$ diverge as $N \to 2$, signaling the presence of logarithms in the correct $N = 2$ calculation.

To write Eq. (5.2) as an equation in C_{vv} and f only, we use the relation $\tilde{C}_{gg} = C_{vv}/\mathcal{D}$, where the denominator $\mathcal{D} = 1 - \frac{2}{N} + \frac{1}{N}\langle\sigma_j\sigma_k|\sigma_j\sigma_k\rangle$. Since a_0 only appears in the combination $\tilde{C}_{gg}$, it drops out of our final equation for C_{vv}. Finally, we calculate

$$\langle\sigma_j\sigma_k|\sigma_j\sigma_k\rangle = \frac{N}{N+2}f^2 F\left(1,1;\frac{N}{2}+2;f^2\right) + \frac{1-f^2}{N}F\left(1,1;\frac{N}{2}+1;f^2\right). \quad (5.10)$$

Expanding Eq. (5.10) in powers of $1/N$ gives

$$\langle\sigma_j\sigma_k|\sigma_j\sigma_k\rangle = f^2 + \frac{1}{N}\frac{1-2f^2}{\gamma^2} + \frac{1}{N^2}\frac{2f^2}{\gamma^2}(3-4f^2) - \frac{1}{N^3}\frac{4f^2}{\gamma^2}(3-14f^2+12f^4) + O(1/N^4). \quad (5.11)$$

Comparison with the $\mathcal{C}_p$ defined above shows that $\mathcal{C}_p \sim O(1/N^p)$ at large N. The $\mathcal{B}_q$ are therefore $O(N^0)$.

B. Similarity solution for C_{vv}

As indicated above, Eq. (5.2) supports the scaling solution $C_{vv} = TL^{2-d}F(r/L)$ for $N > 2$. In this section we derive the ordinary differential equation to be satisfied by F. First, we transform from r to the scaling variable $x = r/L$ and note that $\delta(\mathbf{r}) = \delta(\mathbf{x})/L^d = \delta(x)/L^d\Omega_d x^{d-1}$, where $\Omega_d = 2\pi^{d/2}/\Gamma(d/2)$ is the surface area of a unit sphere in d dimensions. Then we substitute the scaling solution and cancel common factors. Lastly, we recall from Sec. IV that $\mu = \pi S_0/2L^2$ and $L = 2(\Gamma t)^{1/2}$ to get the scaling equation

$$-(d-2)F - xF' = \nabla^2 F + \frac{\pi}{N\mu}\mathcal{B}_1\frac{F}{\mathcal{D}} + \frac{2}{N}\mathcal{B}_2 f'\frac{d}{dx}\left(\frac{F}{\mathcal{D}}\right) - \frac{2}{N^2}\mathcal{B}_3(f')^2\frac{F}{\mathcal{D}} + \frac{N-1}{N}\frac{\delta(x)}{\Omega_d x^{d-1}} \quad (5.12)$$

where a prime indicates a derivative with respect to x.

Consider the scaling equation at large x. Recalling that f decays exponentially at large x, we expand in powers of f^2 to get

$$-(d-2)F - xF' = \nabla^2 F - \frac{\pi}{\mu(N-2)}F + O(Ff^2). \quad (5.13)$$

This has the general solution $F = Ax^{-[2+\pi/\mu(N-2)]}e^{-x^2/2} + Bx^{2-d+\pi/\mu(N-2)}$, where A and B are undetermined constants. We expect that the physical solution decays exponentially and therefore has $B = 0$. We will see that there is a constant in the small x expansion which can be uniquely determined by the requirement that an integration from small to large x matches onto the physical long distance solution.

We now seek the small x expansion of F. At leading order the only terms in Eq. (5.12) to consider are $0 = \nabla^2 F + (1 - \frac{1}{N})\delta(x)/(\Omega_d x^{d-1})$. Recalling that the spherically symmetric Laplacian $\nabla^2 = \frac{1}{x^{d-1}}\frac{\partial}{\partial x}(x^{d-1}\frac{\partial}{\partial x})$ we find $F = -\frac{N-1}{N2\pi}\ln(x)$ in $d = 2$ and $F = \frac{N-1}{N(d-2)\Omega_d}\frac{1}{x^{d-2}}$ in $d > 2$. Since we are considering only $N > 2$ and $d \geq N$, we will further restrict our attention to $d > 2$ in this section.

The calculation of F to next order in x depends upon f. Recall that $f = 1 - \alpha x^2$ at small x, where $\alpha = \pi/(4\mu d)$. We expand Eq. (5.10) for $\langle\sigma_j\sigma_k|\sigma_j\sigma_k\rangle$ and find $\langle\sigma_j\sigma_k|\sigma_j\sigma_k\rangle = 1 - \frac{N-1}{N-2}2\alpha x^2$ with the next order $x^{\min(N,4)}$. Returning to Eq. (5.12), we can calculate F to second order:

$$F = \begin{cases} \left(1-\frac{1}{N}\right)\frac{1}{4\pi}\left(\frac{1}{x}+\nu+\frac{2\alpha}{(N-2)}x\right), & d=3 \\ \left(1-\frac{1}{N}\right)\frac{1}{4\pi^2}\left(\frac{1}{x^2}+\frac{4\alpha}{(N-2)}\ln(x)+\nu\right), & d=4 \\ \left(1-\frac{1}{N}\right)\frac{1}{(d-2)\Omega_d x^{d-2}}\left(1-\frac{2\alpha(d-2)}{(N-2)(d-4)}x^2\right), & d>4. \end{cases} \quad (5.14)$$

The small distance expansion always has an undetermined constant ν entering at $O(x^0)$. This is the first term in the solution of the homogeneous part of Eq. (5.12), which enters with an arbitrary magnitude. As mentioned above, ν can be fixed by the requirement that F decays exponentially at large x. We thus have an eigenvalue problem to be solved by numerical integration for each N and d. We have performed this calculation for the case $N = d = 3$. Figure 1 shows the function $xF(x)$. The corresponding eigenvalue is $\nu(3,3) = -0.1173$.

C. The limits $t \to \infty$ and $N \to \infty$

The short distance singularities in (5.14) are exactly those one expects for Nambu-Goldstone modes in an ordered system. As $t \to \infty$, L diverges and only the leading order term persists. We thus have $C_{vv}(r, t = \infty) = T\frac{N-1}{N(d-2)\Omega_d}\frac{1}{r^{d-2}}$ in $d > 2$. This is the exact $t = \infty$ result [7]. We reserve the case $d = 2$ for Sec. VI.

As $N \to \infty$ we recover the result of Mazenko and Zannetti [16]. Equation (5.12) becomes

$$-(d-2)F - xF' = \nabla^2 F - \frac{\pi}{N\mu}F(1-f^2) - \frac{2}{N}F'ff' + \left(1-\frac{1}{N}\right)\frac{\delta(x)}{\Omega_d x^{d-1}} + O(1/N^2). \quad (5.15)$$

At leading order, the Fourier transform of this equation is $2F + KF' = -K^2F + 1$. This has the solution $F = (1 - e^{-K^2/2})/K^2$.

D. The XY model, $N = 2$

As mentioned above, the term $\langle(\nabla_k\sigma_j\nabla_k v_j)\,\sigma_i|v_i\rangle \sim L^{-2}\ln(L/a)$ for the case $N = 2$. The logarithms originate in the expression $\langle m^{-2}\rangle$, which is $1/(N-2)S_0$ for $N > 2$, but $\ln(L/a)/S_0 + O(1)$ for $N = 2$. The only terms that differ from those in Sec. V A are $\mathcal{B}_1 = -\ln(L/a)/2 + O(1, \ln x)$ and $\mathcal{B}_3 = \gamma^2[\ln(L/a)/2 + O(1, \ln x)]$. For $r \gg a$, Eq. (5.2) becomes

$$\frac{1}{2}\frac{\partial C_{vv}}{\partial t} = \Gamma\Big(\nabla_r^2 C_{vv} + \frac{C_{vv}}{2\mathcal{D}}\frac{\ln(L/a)}{L^2}\left(\frac{\pi}{2\mu} + \frac{\gamma^2}{2}(\nabla_x f)^2\right) + \frac{T}{2}\delta(\mathbf{r})\Big) + O(L^{-2}C_{vv}), \tag{5.16}$$

where f and γ are functions of the scaling variable $x = r/L$, as before.

We can still find a scaling solution for C_{vv}, with the surprising feature that the characteristic length is logarithmically smaller than L. We find $C_{vv} = Tl^{2-d}F(r/l)$ where $l = L/[\ln(L/a)]^{1/2}$. In terms of the new scaled variable $y = r/l$ the scaling equation simplifies to

$$0 = \nabla_y^2 F - \left(\frac{\pi}{2\mu} + \alpha\right)F + \frac{\delta(y)}{2\Omega_d y^{d-1}} + O(F/\ln(L/a)) \tag{5.17}$$

where we have replaced the functions of x in Eq. (5.16) by their values at $x = 0$. This equation can be solved exactly in Fourier space to give $F(K) = \frac{1}{2}(K^2 + m^2)^{-1}$, where $m^2 = \pi/2\mu + \alpha$ and the scaling variable is $K = kl$. The expected corrections are of relative order $1/\ln(L/a)$.

VI. $C_{\psi\psi}$ TO ORDER T AND THE CASE $D = 2$

We have avoided until now the issue of higher order corrections to our approximate separation $\vec{\psi} = \vec{\sigma} + \vec{v}$. To satisfy $\psi^2 = 1$ to first nontrivial order in T, the only consistent substitution is $\vec{\psi} = (1 - v^2/2)\vec{\sigma} + \vec{v}$. With this we can calculate the order parameter correlation function to first order in the temperature $C_{\psi\psi} = (1 - \langle v^2\rangle)C_{\sigma\sigma} + C_{vv} + O(T^2)$.

Consider the case $d > 2$. The amplitude of thermal fluctuations $\langle v^2\rangle = NC_{vv}(a) = T\frac{N-1}{(d-2)\Omega_d a^{d-2}} - O(TL^{2-d})$ is asymptotic to a constant. Inserting the scaling forms, we have $C_{\psi\psi} = (1 - \langle v^2\rangle)G(r/L) + TL^{2-d}F(r/L) + O(T^2)$ (for the case $N = 2$, replace L by l in the last term). Note that the relative amplitude of the spin wave correlation function diminishes as L^{2-d}. This is in agreement with the expectation that T is an irrelevant variable in $d > 2$. As a consequence, it will be extremely difficult to determine F by either experiment or simulation.

Now consider the case $d = d_c = 2$, at the lower critical dimension of the NLS model. Since we have been considering only $N \leq d$, we restrict our attention to the XY model. The quantity $\langle v^2\rangle = T\ln(l/a)/2\pi + O(T)$ diverges logarithmically with l. As the system coarsens, we thus expect that the thermal fluctuations will increase in amplitude until v is comparable to σ, at which point our approximation $v \ll \sigma$ will fail. This is a reminder that thermal fluctuations destroy the long-range order in two dimensions, with the surprising implication that l plays the role of an effective system size.

It is instructive to define the length L^* at which $\langle v^2\rangle = 1$. We find $L^* = a(2\pi/T)^{1/2}\exp(-2\pi/T)$. This is in remarkable qualitative agreement with the average *equilibrium* separation between defect-antidefect pairs at low temperatures as estimated by Kosterlitz and Thouless $L_{\rm KT} \approx a(1/\pi T)^{1/2}\exp(-\pi^2/2T)$ [18]. This is encouraging, especially since the $T^{-1/2}$ factor arises in our theory due to the logarithmic difference between L and l.

We thus make the prediction that the XY model in two dimensions will exhibit qualitatively normal coarsening for $L \ll L_{\rm KT}(T)$. As L increases, the amplitude of thermal fluctuations will increase as $\langle v^2\rangle \approx T\ln(l/a)/2\pi$. It is only when $L \approx L_{\rm KT}(T)$ and $\langle v^2\rangle \approx 1$ that thermal fluctuations are large enough to create defect-antidefect pairs in significant numbers and we expect a crossover to equilibrium behavior. Until then, pair creation is suppressed.

This prediction is supported in part by simulations of the XY model in two dimensions reported by Yurke *et al.* [10]. They observed qualitatively normal defect coarsening at a range of temperatures below $T_{\rm KT}$. The primary difference between their results and the theory presented here was an apparent logarithmic correction to the growth law $L \sim [t/\ln(t)]^{1/2}$. This is due to a renormalization of Γ which our theory cannot account for. They limited their observations to temperatures for which $L_{\rm KT}$ was greater than their system size, so they do not illuminate the crossover regime $L \approx L_{\rm KT}$. It would be very instructive to examine this regime further.

VII. CONCLUSION

In this paper we have presented a calculation of the order parameter correlation function for the defect coarsening problem as described by the NLS model. We focused on the case $N \leq d$ and low temperatures. We used the approximate separation of the time scales associated with thermal fluctuations and defect coarsening to motivate the decomposition of the order parameter $\vec{\psi} = \vec{\sigma} + \vec{v}$, slow and fast modes respectively. Although the equations of motion for σ and v are introduced in a somewhat *ad hoc* manner, they successfully reproduce much of the phenomenology of defect coarsening.

We used the Gaussian closure approximation to derive an ordinary differential equation for the scaling solution $C_{\sigma\sigma}(r,t) = G(r/L)$. A second Gaussian assumption was introduced in order to calculate the fast-mode correlation function C_{vv}. We found that C_{vv} has a scaling solution $C_{vv}(r,t) = Tl^{2-d}F(r/l)$ for $N = 2$ and $C_{vv}(r,t) = TL^{2-d}F(r/L)$ for $N > 2$ in $d \geq N$. The main result of this paper is an ordinary differential equation whose solution is the scaling function $F(x)$. We calculated this solution analytically for $N = 2$ and numerically for $N = d = 3$.

In $d > 2$ dimensions, we found that the assymptotic order parameter correlation function is independent of temperature up to a multiplicative constant, in agreement with the belief that temperature is an irrelevant variable for these systems. Lastly, we considered the case of the XY model in $d = d_c = 2$. Our theory makes several qualitative predictions for this system. Most notable is the prediction that defect-antidefect pair creation will be suppressed until $L \approx L_{\mathrm{KT}}(T)$, where $L_{\mathrm{KT}}(T)$ is the average separation between pairs in equilibrium.

There are several avenues of research suggested by the results in this paper. (1) Can this phenomenological calculation be systematically improved? (2) Is the small difference between f_{NLS} and f_{TDGL} indicative of a genuine violation of universality or is it a relic of the Gaussian approximation? (3) Can these results be extended to the case $N > d$, where topological textures can play an important role? (4) To what extent can $F(x)$ be determined empirically? And lastly, this paper clearly indicates the need for a systematic study of the crossover from coarsening to equilibrium behavior in the two dimensional XY model at $T < T_{\mathrm{KT}}$.

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