Asymptotic Structure Factor and Power-Law Tails for Phase Ordering in Systems with Continuous Symmetry

A. J. Bray[(1)] and Sanjay Puri[(2),(a)]
[(1)]Department of Theoretical Physics, The University, Manchester M13 9PL, United Kingdom
[(2)]Institut für Physik, Johannes Gutenberg Universität Mainz, D6500 Mainz, Germany
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We compute the asymptotic structure factor $S_{\mathbf{k}}(t)$ $[=L(t)^d g(kL(t))$, where $L(t)$ is a time-dependent characteristic length scale and d is the dimensionality] for a system with a nonconserved n-component vector order parameter quenched into the ordered phase. The well-known Ohta-Jasnow-Kawasaki-Yalabik-Gunton result is recovered for $n=1$. The scaling function $g(x)$ has the large-x behavior $g(x)\sim x^{-(d+n)}$, which includes Porod's law (for $n=1$) as a special case.

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The phase ordering dynamics of a system quenched into the ordered phase from a high-temperature homogeneous state is an area of continuing interest [1]. The fascination of this field is due in great part to the scaling regime which emerges in the late stages of growth. There is overwhelming experimental and numerical support for the "scaling hypothesis," according to which the structure of the order-parameter field at time t after the quench is characterized by a single length scale $L(t)$. For example, when the order parameter is scalar, $L(t)$ measures the size of the ordered domains that have developed at time t. Much recent interest has also centered on phase ordering in systems with more complicated internal symmetries such as n-component vector models [2,3] (including superconductors) and the nematic phase of liquid crystals [4]. However, little is known about the analytic form of the structure factor in such systems. The only analytic result we are aware of is due to Puri [5], who has obtained an asymptotic form for the case of a nonconserved two-component order parameter with O(2) symmetry, but did not investigate the tail behavior. In this Letter we derive, for the first time, the structure factor for a nonconserved n-component vector order parameter with O(n) symmetry. Our approach is based on a singular perturbation expansion proposed by Suzuki [6] and extended by Kawasaki, Yalabik, and Gunton [7].

The most important consequence of the existence of a characteristic length scale $L(t)$ is that the order-parameter correlation function

$$C(\mathbf{r},t)=\langle\vec{\phi}(\mathbf{x},t)\cdot\vec{\phi}(\mathbf{x}+\mathbf{r},t)\rangle \tag{1}$$

has the scaling form $C(\mathbf{r},t)\equiv C(r,t)=f(r/L(t))$ (assuming isotropy). The angular brackets in (1) indicate an average over the ensemble of possible initial conditions. Of greater experimental interest is the Fourier transform of $C(\mathbf{r},t)$, the time-dependent structure factor $S_{\mathbf{k}}(t)$, which is directly measurable in scattering experiments. The corresponding scaling form for $S_{\mathbf{k}}(t)$ is

$$S_{\mathbf{k}}(t)=L(t)^d g(kL(t)), \tag{2}$$

where d is the dimensionality. In this Letter, we obtain a closed-form expression for the real-space scaling function $f(y)$ for the case of a nonconserved n-component vector order parameter with O(n) symmetry. We find that the corresponding scaling function in momentum space has the asymptotic behavior $g(x)\sim x^{-(d+n)}$ for large x $[=kL(t)]$, i.e., in the tail. For the special case when $n=1$, our closed expression for $f(y)$ reduces to the well-known result of Kawasaki, Yalabik, and Gunton [7] and Ohta, Jasnow, and Kawasaki [8]. Furthermore, the so-called Porod's law [9] for the one-component system $[g(x)\sim x^{-(d+1)}]$ is recovered from our general form. The explicit n dependence of the tail exponent in the general result is remarkable and unexpected: Naively, one might have anticipated the same behavior for all systems with continuous symmetry ($n\geq 2$). Possible experimental consequences of our predictions will be discussed.

The equation of motion for the nonequilibrium dynamics of a nonconserved n-component vector order parameter with O(n) symmetry $\vec{\phi}(\mathbf{r},t)$ reads (in dimensionless variables) [10]

$$\frac{\partial\vec{\phi}}{\partial t}=\vec{\phi}-(\vec{\phi}^2)\vec{\phi}+\nabla^2\vec{\phi}. \tag{3}$$

The absence of a thermal noise term in (3) indicates that we are working at temperature $T=0$: Temperature is an "irrelevant variable" for phase ordering dynamics (provided T is less than the critical temperature T_c). Equation (3) has to be supplemented by an initial condition on $\vec{\phi}$. We make the reasonable assumption that the components of $\vec{\phi}(\mathbf{r},0)$ are independent Gaussian random variables with $\langle\phi_i(\mathbf{r},0)\rangle=0$, where ϕ_i is a Cartesian component of $\vec{\phi}$. The singular perturbation technique applied to (3) involves an iterative expansion in terms of the solution of the linear part of (3), viz., the "noninteracting" solution

$$\vec{\phi}_0(\mathbf{r},t)=\exp\{t(1+\nabla^2)\}\vec{\phi}(\mathbf{r},0). \tag{4}$$

Since the linear solution diverges exponentially with t, each term in the perturbation expansion is more divergent than the last. In the singular perturbation method [6,7], the divergence is handled by retaining only the dominant divergent contribution at each order. In this limit, every diagram at a given order yields the same, easily evaluated, contribution. Applying this technique to (3) gives the result [11]

$$\vec{\phi}(\mathbf{r},t)=\frac{\vec{\phi}_0(\mathbf{r},t)}{[1+\vec{\phi}_0(\mathbf{r},t)^2]^{1/2}}\rightarrow\frac{\vec{\phi}_0(\mathbf{r},t)}{|\vec{\phi}_0(\mathbf{r},t)|}, \tag{5}$$

where the final expression is valid as $t\rightarrow\infty$.

It should be stressed that we do not believe (5) to be exact. Rather, (4) and (5) capture the essential features of the assembly of topologically stable singularities seeded by the initial conditions. By singularities we mean the set of points at which $\vec{\phi}(\mathbf{r},t)=0$. Such points form walls ($n=1$), strings ($n=2$), or hedgehogs ($n=3$), and their density decreases with time as $L(t)^{-n}$.

It is now a straightforward (though lengthy) procedure [11] to obtain from (4) and (5) the real-space correlation function $C(r,t)=\langle\vec{\phi}(\mathbf{x}_1,t)\cdot\vec{\phi}(\mathbf{x}_2,t)\rangle$, where $r=|\mathbf{x}_1-\mathbf{x}_2|$. Using the integral representation

$$|\vec{\phi}_0|^{-1}=\int_{-\infty}^{\infty}(d\theta/\sqrt{2\pi})\exp(-\theta^2\vec{\phi}_0^2/2)$$

for each of the factors in $C(r,t)$ yields

$$C(r,t)=\int_{-\infty}^{\infty}\frac{d\theta}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{d\psi}{\sqrt{2\pi}}\langle\vec{\phi}_0(1)\cdot\vec{\phi}_0(2)\exp\{-(\theta^2/2)\vec{\phi}_0(1)^2-(\psi^2/2)\vec{\phi}_0(2)^2\}\rangle, \tag{6}$$

where $\vec{\phi}_0(1)\equiv\vec{\phi}_0(\mathbf{x}_1,t)$, etc. Now, the different Cartesian components of $\vec{\phi}_0(\mathbf{r},t)$ are independent random variables according to (4). In fact, if we let x and y stand for a given component (say the first) of $\vec{\phi}_0(1)$ and $\vec{\phi}_0(2)$, then from the Gaussian property one has the joint probability distribution

$$\rho(x,y)=\frac{1}{2\pi\sigma^2(1-\gamma^2)^{1/2}}\exp\left(-\frac{x^2+y^2-2\gamma xy}{2\sigma^2(1-\gamma^2)}\right), \tag{7}$$

where

$$\sigma^2=\langle x^2\rangle=\langle y^2\rangle,\quad \gamma=\langle xy\rangle/\langle x^2\rangle. \tag{8}$$

The parameter γ carries the scaling dependence on r and t: From (4), it follows that

$$\gamma=\exp\{-r^2/2L(t)^2\}, \tag{9}$$

where we have introduced $L(t)=(4t)^{1/2}$ in anticipation of its emergence as the characteristic length scale. In particular, $\gamma\rightarrow 1$ for $r\ll L(t)$, while $\gamma\rightarrow 0$ for $r\gg L(t)$.

Using the statistical independence of the different Cartesian components of $\vec{\phi}_0(\mathbf{r},t)$, the average over initial conditions can be carried out separately for each component. After some algebra, the result reduces to

$$C(r,t)=n\gamma\int_{-\infty}^{\infty}\frac{d\theta}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{d\psi}{\sqrt{2\pi}}[1+\theta^2+\psi^2+(1-\gamma^2)\theta^2\psi^2]^{-(n+2)/2}. \tag{10}$$

The ψ integral can be evaluated by elementary means. After changing variables to $x=\theta^2$ we obtain the final closed-form result [12,13],

$$\begin{aligned}C(r,t)&=\frac{n\gamma}{2\pi}B\left(\frac{n+1}{2},\frac{1}{2}\right)\int_0^{\infty}dx\,x^{-1/2}(1+x)^{-(n+1)/2}(1+[1-\gamma^2]x)^{-1/2}\\&=\frac{n\gamma}{2\pi}\left[B\left(\frac{n+1}{2},\frac{1}{2}\right)\right]^2F\left(\frac{1}{2},\frac{1}{2};\frac{n+2}{2};\gamma^2\right),\end{aligned} \tag{11}$$

where $B(x,y)\equiv\Gamma(x)\Gamma(y)/\Gamma(x+y)$ is the beta function, and $F(a,b;c;z^2)$ is the hypergeometric function.

Several limiting cases of (11) are of interest. For $n=1$, the identity

$$F(\tfrac{1}{2},\tfrac{1}{2};\tfrac{3}{2};z^2)=\arcsin(z)/z$$

gives the well-known result [7,8] $C(r,t)=(2/\pi)\times\arcsin(\gamma)$, with γ given by (9). For $n\rightarrow\infty$, the integral leading to (11) is dominated by small x [i.e., $x=O(1/n)$], so the final factor in the integrand can be replaced by unity to leading order. This gives $C(r,t)=\gamma$, in agreement with the exact solution in this limit [3]. For general n one can extract simple forms for large and small values of the scaling variable $r/L(t)$, i.e., the limits $\gamma\rightarrow 0$ and $\gamma\rightarrow 1$. For $\gamma\rightarrow 0$, $F(a,b;c;0)=1$ gives immediately

$$C(r,t)\rightarrow(n\gamma/2\pi)[B((n+1)/2,1/2)]^2,$$

i.e., $C(r,t)\sim\exp[-r^2/2L(t)^2]$ for $r\gg L(t)$. The limit $\gamma\rightarrow 1$ is much more interesting because it turns out that, for any n, the scaling function $f(y)$ defined by $C(r,t)=f(r/L(t))$ is *nonanalytic in* y *at* $y=0$. It is this nonanalyticity in $f(y)$ which leads to the power-law tail in its Fourier transform, the scaling function $g(x)$ of (2). As an example, the $n=1$ scaling function $f(y)=(2/\pi)\times\arcsin\{\exp(-y^2/2)\}$ has the small-y behavior $f(y)\simeq 1$

$-(2/\pi)y$. It follows that $g(x)\sim x^{-(d+1)}$ for large x, which is the well-known Porod's law [9]. For general n, we rewrite Eq. (11) in a form more convenient for considering the limit $\gamma\to 1$. Using standard transformation formulas for the hypergeometric function [13], (11) can be recast in the form

$$C(r,t)=\gamma F\left[\frac{1}{2},\frac{1}{2};\frac{2-n}{2};1-\gamma^2\right]+\frac{n\gamma}{2\pi}\frac{\Gamma^2((n+1)/2)\Gamma(-n/2)}{\Gamma((n+2)/2)}(1-\gamma^2)^{n/2}F\left[\frac{n+1}{2},\frac{n+1}{2};\frac{n+2}{2};1-\gamma^2\right]. \quad (12)$$

For $y\to 0$, $1-\gamma^2\equiv 1-\exp(-y^2)\simeq y^2$. Considering first the case where n is an odd integer, it is clear from (12) that, since $F(a,b;c;z^2)$ has a power-series expansion in z^2 for small z, the leading nonanalyticity in y comes from the second term in (12), which yields a contribution of order y^n. [Since $C(\mathbf{r},t)$ depends only on $r\equiv|\mathbf{r}|$, analyticity in $\mathbf{r}$ would require an expansion in even powers of r.] Specifically, this singular part of $C(r,t)$ is

$$C_{\text{sing}}(r,t)=\frac{n}{2\pi}\frac{\Gamma^2((n+1)/2)\Gamma(-n/2)}{\Gamma((n+2)/2)}y^n. \quad (13)$$

When n is an even integer, the two terms in (12) combine to give a leading singularity of the form $y^n\ln y$. As a matter of fact, Mondello and Goldenfeld [2] have numerically observed that, for $n=d=2$, $1-f(y)\sim y^\phi$ for $y\ll 1$, with $\phi\simeq 1.6$. Given a limited range of y values, this is compatible with our analytic form for $n=2$, $d=2$, viz., $1-f(y)\sim y^2(1/y)$. It turns out that the tail behavior in $g(x)$ for even n is the same as that derived below for odd n [11], so for the moment we will confine ourselves to the case where n is odd.

From (13), simple power counting yields $g(x)\sim x^{-(d+n)}$ for the large-x behavior of $g(x)$. To determine the coefficient we assume

$$g(x)\to A(n,d)x^{-(d+n)},\quad x\to\infty \quad (14)$$

and Fourier transform $g(x)$ to get the leading singular term in $f(y)$. Comparing the result with (13) confirms (14) and gives

$$A(n,d)=2^n(4\pi)^{d/2}\frac{n}{2\pi}\frac{\Gamma^2((n+1)/2)\Gamma((d+n)/2)}{\Gamma((n+2)/2)}. \quad (15)$$

We note that the final result (15) is smooth as n passes through the even integers. In fact, one can confirm that (14) and (15) hold for general n. Equations (11) and (14) constitute the central results of this Letter.

Qualitatively, Porod's law for the one-component case can be understood as the consequence of sharp interfaces between domains [9]. Clearly, systems with continuous symmetry do not have sharp interfaces. Naively, one might expect that the absence of sharp interfaces in systems with O(n) symmetry would result in exponentially decaying tails for the scaled structure factor, as in the $n\to\infty$ limit [3]. Our results indicate that the tail of the n-component structure factor has the remarkably simple power-law form (14). For the physically important case $n=2$, $d=2$, we can construct a simple heuristic argument [11] which recovers (14) by exploring the vortex configuration. This argument generalizes to any case where the system has topological singularities, i.e., for $n\le d$. However, the considerations leading to (14) suggest that the tail behavior is independent of the existence of topological singularities in the system. We are presently investigating the role of topological singularities in fixing a power-law behavior like (14) for the tail. We have already noted that, for $n\le d$, (4) and (5) generate the topologically stable field configurations (walls, strings, and hedgehogs) that can account for (14). We suspect that (14) may be spurious for $n>d$, being associated with topologically unstable singularities generated by (4) and (5) but absent from the full dynamics (3). For $d=1$, $n=2$, for example, the structure factor is known to have a Gaussian tail [14]. Of course, it should be kept in mind that most cases of physical interest are described by $n\le d$ and, hence, do have topological singularities present.

Finally we discuss the experimental relevance of our results. Most experiments so far have concentrated on the case with a scalar order parameter. However, a variety of important experimental systems, e.g., superconductors [described by the two-component case of (3)] and nematic liquid crystals [4], are described by nonscalar order parameters. Related models have been used in an attempt to understand the large-scale structure of the Universe [15]. We urge experimentalists to investigate the short-wavelength behavior of scattering data from systems with continuous symmetries as a test of our predictions.

To summarize, we have derived an asymptotic form for the structure factor for nonconserved order-parameter systems with O(n) symmetries. The most remarkable feature of our result is the emergence of a simple power-law form for the tail of the structure factor in momentum space, viz., $g(x)\sim x^{-(d+n)}$. This is probably related to the existence of topological defects in these systems and we are currently investigating the connection. We expect that the tail behavior reported here is more general than the methods used to derive it would suggest. Specifically, as is known to be true for the one-component case, we believe that a similar tail behavior will be seen in conserved-order-parameter systems with O(n) symmetries.

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Note added.— After this Letter was submitted for publication, we received a preprint from Toyoki [16], who has derived equivalent results by similar methods. Numerical simulations by Toyoki [17], on $d=3$ systems with

$n = 2,3$, give results fully consistent with the prediction of Eq. (14).

[a]Permanent address: School of Physical Sciences, Jawaharlal Nehru University, New Delhi 110067, India.

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