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Universal amplitudes of power-law tails in the asymptotic structure factor of systems with topological defects

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We compute the asymptotic structure factor $S(\mathbf{k},t)$ of the O(n) model for $n \leq d$, where d and n are the dimensions of space and of the order parameter, respectively. Topological defects in the field lead to the power-law tail $S(\mathbf{k},t) = A(n,d)\rho(t)k^{-(d+n)}$, where ρ is the defect density. The amplitude $A(n,d)$ is calculated exactly using purely geometrical arguments based on the defect field.

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In recent years there has been growing interest in the phase ordering kinetics of systems with continuous, as well as discrete, symmetry [1–7]. Interest has been focused primarily on the scaling regime which emerges at long times after a quench into the ordered phase from the high-temperature homogeneous phase [8,9].

The key experimental probe is the structure factor $S(\mathbf{k},t)$, which is directly measurable in small-angle scattering experiments. The structure factor and its Fourier transform, the pair-correlation function $C(\mathbf{r},t)$, are defined in terms of the order-parameter field $\vec{\phi}(\mathbf{x},t)$ (taken to be an n-component vector) as

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

where $\vec{\phi}_{\mathbf{k}}(t)$ is a Fourier component of $\vec{\phi}(\mathbf{x},t)$ and angular brackets indicate an average over initial conditions.

The form of $S(\mathbf{k},t)$ is usually discussed using a scaling phenomenology [9] in which the structure factor and its Fourier transform exhibit the scaling forms

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

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

where $L(t)$ is a characteristic scale which emerges at late times after the quench. Although the validity of this "scaling hypothesis" has not been verified from first principles (except in some simple limits [10]), it is supported by a large amount of experimental and simulational evidence.

A recent approximate calculation of $S(\mathbf{k},t)$ for a nonconserved order parameter (model A), starting from the time-dependent Ginzburg-Landau equation, predicts [3] that $S(\mathbf{k},t)$ should exhibit a *power-law tail* of the form $L(t)^{-n}k^{-(d+n)}$ for $kL(t) \gg 1$. While the origin of this tail, whose existence is in accord with simulation results [2,4,11], was not transparent either from the original work [3] or subsequent variations [4–6], recent work [12] has shown that it can be understood simply as a consequence of the existence of topological defects in the order-parameter field. Thus the $k^{-(d+n)}$ tail is a natural generalization of Porod's law [13], the $k^{-(d+1)}$ tail observed for a scalar order parameter (i.e., $n=1$). The latter has long been understood to follow from the presence of sharp domain walls separating domains of the two pure phases, a domain wall being the simplest topological defect. For $n>1$, the topological defects are vortices ($d=2$, $n=2$), strings ($d=3$, $n=2$, also called vortex lines), or monopoles ($d=3$, $n=3$, also called hedgehogs). Such localized defects have a core where the order parameter vanishes, and only exist for $n \leq d$. Extended defects known as *textures* can also exist for systems with $n=d+1$, but this case is more complex and will not be considered explicitly here.

Assuming that the scaling hypothesis holds, it is instructive to consider how the defect density ρ_{def} depends on the characteristic scale $L(t)$. By ρ_{def} we mean, for example, the area of domain wall ($n=1$), the length of string ($n=2$), or the number of monopoles ($n=3$), per unit volume. The dimension of ρ_{def} is thus (length)$^{-n}$ in all cases, and ρ_{def} therefore scales as $L(t)^{-n}$.

This suggests the following simple derivation [12] of the power-law tail in $S(\mathbf{k},t)$. For $kL(t) \gg 1$, the structure factor probes length scales short compared to the characteristic distance [$\sim L(t)$] between defects. In this regime, therefore, the total structure factor is essentially a one-defect property, and $S(\mathbf{k},t)$ should be proportional to the defect density ρ_{def}, which itself scales as $L(t)^{-n}$. Demanding that the scaling form (3) reproduce this factor requires that the scaling function $g(y)$ behave as $g(y) \sim y^{-(d+n)}$ for $y \gg 1$, which is the desired result.

While this heuristic argument is very simple and persuasive, it hides the underlying mechanism that gives rise to the tail, namely, the long-range distortion of the order-parameter field by topological defects. The latter is the subject of this paper. We show by explicit calculation that the presence of defects leads to a *singular* short-distance behavior in the real-space correlation function $C(\mathbf{r},t)$, through a term of the form $|\mathbf{r}|^n$ for n odd (or noninteger, in a continuation of the theory to real n), and $|\mathbf{r}|^n \ln|\mathbf{r}|$ for n even. This in turn implies, through simple power counting, the power-law tail $k^{-(d+n)}$ in $S(\mathbf{k},t)$. The final result for the tail has the form

$$S(\mathbf{k},t) = A(n,d)\rho_{\text{def}}k^{-(d+n)} . \tag{4}$$

The amplitude $A(n,d)$ can be calculated exactly. It is

$$A(n,d) = \frac{1}{\pi}(4\pi)^{(d+n)/2}\frac{\Gamma^2((n+1)/2)\Gamma(d/2)}{\Gamma(n/2)} . \tag{5}$$

This result is consistent with the scaling argument given above, but is more general. In particular, it does not require scaling to hold. We note that this exact result provides both a powerful test of approximate theories and an experimental tool to measure $\rho_{\rm def}$.

To derive Eqs. (4) and (5), we will start with the conceptually simplest case of point defects, $n=d$. (For $n=d=2$, this approach was discussed briefly in Ref. [6].) Consider the field $\vec{\phi}$ at points $\mathbf{x}$ and $\mathbf{x}+\mathbf{r}$ in the presence of a point defect at the origin. We consider the case where $|\mathbf{x}|$, $|\mathbf{x}+\mathbf{r}|$, and $|\mathbf{r}|$ are all small compared to a typical interdefect distance L, but large compared to the defect core size. Then the field at the points $\mathbf{x}$ and $\mathbf{x}+\mathbf{r}$ is saturated in length, and not significantly distorted by the presence of other defects. Moreover, the field can be taken, up to a global rotation, to be directed radially outward from the origin. Thus

$$\vec{\phi}(\mathbf{x})\cdot\vec{\phi}(\mathbf{x}+\mathbf{r})=\frac{\mathbf{x}\cdot(\mathbf{x}+\mathbf{r})}{|\mathbf{x}||\mathbf{x}+\mathbf{r}|}\ , \tag{6}$$

where we have taken the equilibrium value of $|\vec{\phi}|$ to be unity, and we are ignoring thermal fluctuations, i.e., working at $T=0$. This restriction will be relaxed below. With $\mathbf{r}$ held fixed we average (6) over all possible relative positions of the point defect, i.e., over all values of $\mathbf{x}$ within a volume of order L^n around the pair of points, with the appropriate probability density $\rho_{\rm def}$. Focusing on the singular part of the correlation function we obtain

$$C_{\rm sing}(\mathbf{r},t)=\rho_{\rm def}\int^L d^n x\left[\frac{\mathbf{x}\cdot(\mathbf{x}+\mathbf{r})}{|\mathbf{x}||\mathbf{x}+\mathbf{r}|}-(\text{analytic terms})\right]\ . \tag{7}$$

The (analytic terms) in (7) are included so that the $\mathbf{x}$ integral may be extended over all space. We include as many terms in the expansion of (6) in powers of $\mathbf{r}$ as are necessary to ensure the convergence of the integral (7). When n is even, there is a residual logarithmic singularity. This case can be retrieved from the general n result by taking a suitable limit (see below). For brevity we will not write the analytic terms in (7) explicitly: their presence should be understood in what follows.

Using the integral representation

$$|\mathbf{x}|^{-1}=\int_0^\infty (dy/\sqrt{\pi y})\exp(-yx^2)$$

for each of the factors in the integrand in (7) yields

$$C_{\rm sing}(\mathbf{r},t)=\frac{\rho_{\rm def}}{\pi}\int_0^\infty\frac{dy\,dz}{\sqrt{yz}}\exp(-zr^2)\times\int d^n x\,\mathbf{x}\cdot(\mathbf{x}+\mathbf{r})\times\exp(-yx^2-2z\mathbf{x}\cdot\mathbf{r}-zx^2)\ . \tag{8}$$

We now make the following change of variables: $y=u/v$, $z=u/(1-v)$, and $\mathbf{x}=\sqrt{v(1-v)}\mathbf{x}'-v\mathbf{r}$. After some algebra (8) becomes, suppressing the prime,

$$C_{\rm sing}=\frac{\rho_{\rm def}}{\pi}\int_0^1 dv\,[v(1-v)]^{(n-1)/2}\times\int_0^\infty du\,\exp(-ur^2)\times\int d^n x\,(x^2-r^2)\exp(-ux^2)\ . \tag{9}$$

The integrals over v and x can now be evaluated. The result is

$$C_{\rm sing}=\pi^{n/2-1}B\left(\frac{n+1}{2},\frac{n+1}{2}\right)\rho_{\rm def}\times\int_0^\infty du\,u^{-n/2}\exp(-ur^2)\left(\frac{n}{2u}-r^2\right)\ , \tag{10}$$

where $B(x,y)$ is the beta function. Reinstating the analytic terms from (7) requires us to subtract from the integrand of (10) as many terms of the expansion in powers of r^2 as are required to converge the integral at small u. The u integral can then be evaluated in terms of Γ functions. The final result is

$$C_{\rm sing}=n\pi^{n/2-1}B\left(\frac{n+1}{2},\frac{n+1}{2}\right)\Gamma\left(-\frac{n}{2}\right)\rho_{\rm def}|\mathbf{r}|^n\ . \tag{11}$$

The pole in the $\Gamma(-n/2)$ factor for even values of n signals a contribution of the form $|\mathbf{r}|^n\ln(|\mathbf{r}|/L)$ to $C_{\rm sing}$ for those cases. To see how this comes about, we set $n=2m+\epsilon$ in (11), and take the limit $\epsilon\to 0$. The leading pole contribution, proportional to $\epsilon^{-1}(r^2)^m$, is analytic in $|\mathbf{r}|$ and therefore does not contribute to $C_{\rm sing}$. The O(1) term (in the expansion in powers of ϵ) generates the logarithmic correction from the expansion of $|\mathbf{r}|^{2m+\epsilon}$. Since, however, the result in Fourier space is completely smooth as a function of n, we will not give a separate detailed discussion for even n.

Using the above result for point defects we can generalize our calculation to all $n\le d$. For $n<d$, the defects are spatially extended, with dimension $(d-n)$. An important observation is that, since the lengths $|\mathbf{x}|$, $|\mathbf{x}+\mathbf{r}|$, and $|\mathbf{r}|$ of interest are small compared to the scale L that characterizes the defect structure, the defects can be taken to be flat on these short scales, i.e., a domain wall can be treated locally as a flat plane, a string as a straight line, etc. The $\mathbf{x}$ vector is then taken to be directed normal to the defect. The key idea is then to resolve the d-component $\mathbf{r}$ vector into two vectors $\mathbf{r}_\parallel$ and $\mathbf{r}_\perp$. The $\mathbf{r}_\parallel$ vector is a $(d-n)$-dimensional vector parallel to the defect, whose orientation is specified by the first $(d-n)$ polar angles, while $\mathbf{r}_\perp$ is an n-component vector lying in the n-dimensional subspace perpendicular to the defect, with orientation specified by the remaining $n-1$ polar angles. If we keep $\mathbf{r}_\parallel$ fixed (i.e., $\theta_1,\theta_2,\ldots,\theta_{d-n}$ are kept fixed), and average over the remaining $n-1$ angles associated with the orientation of $\mathbf{r}_\perp$, then we have effectively reduced the problem to one of point defects in the n-dimensional subspace, with $\mathbf{r}_\perp$ playing the role played by $\mathbf{r}$ in the previous calculation. The result of averaging over the orientation of $\mathbf{r}_\perp$ is then given by (11), with $|\mathbf{r}|^n$ replaced by $|\mathbf{r}_\perp|^n$.

The final step is to average over the orientation of $\mathbf{r}$, i.e., to average over polar angles $\theta_1,\theta_2,\ldots,\theta_{d-n}$. This gives, for general $n\le d$,

$$C_{\rm sing}=n\pi^{n/2-1}B\left(\frac{n+1}{2},\frac{n+1}{2}\right)\Gamma\left(-\frac{n}{2}\right)\rho_{\rm def}\langle|\mathbf{r}_\perp|^n\rangle\ , \tag{12}$$

where $\langle\ \rangle$ indicates the angular average. Evaluating the latter is straightforward, and gives

$$\langle |\mathbf{r}_\perp|^n \rangle = \langle \sin^n\theta_1 \sin^n\theta_2 \cdots \sin^n\theta_{d-n} \rangle |\mathbf{r}|^n = \frac{\Gamma(d/2)\Gamma(n)}{\Gamma((d+n)/2)\Gamma(n/2)} |\mathbf{r}|^n . \quad (13)$$

Putting (13) into (12) and using $B(x,y)=\Gamma(x)\Gamma(y)/\Gamma(x+y)$, where $\Gamma(x)$ is the gamma function, gives the final result

$$C_{\rm sing} = \pi^{n/2-1} \frac{\Gamma(-n/2)\Gamma(d/2)\Gamma^2((n+1)/2)}{\Gamma((d+n)/2)\Gamma(n/2)} \rho_{\rm def} |\mathbf{r}|^n . \quad (14)$$

We remarked in the preceding section that for even n the leading singularity is the form of $r^n \ln r$, but the Fourier transform $S(\mathbf{k},t)$ of $C_{\rm sing}(\mathbf{r},t)$ has the same form for even, odd, and real n, so we will not consider the even n case explicitly.

It remains to Fourier transform (14) to obtain the tail of the structure factor. Simple power counting on (14) gives immediately the power-law tail $S(\mathbf{k},t) \sim k^{-(d+n)}$. To derive the amplitude we exploit the integral representation

$$\Gamma(-n/2)|\mathbf{r}|^n = \int_0^\infty du\, u^{-n/2-1} \{\exp(-ur^2) - (\text{analytic terms})\} , \quad (15)$$

where (analytic terms) indicates, once more, as many terms in the expansion of $\exp(-ur^2)$ as are necessary to converge the integral. These terms will not contribute to the tail of the Fourier transform, and can be dropped once the transform has been taken. The Fourier transform of (15) is, therefore,

$$\int_0^\infty du\, u^{-n/2-1} \int d^d r \exp(-ur^2 - i\mathbf{k}\cdot\mathbf{r}) = \pi^{d/2} \int_0^\infty du\, u^{-(d+n)/2-1} \exp(-k^2/4u) = \pi^{d/2} \Gamma\left[\frac{d+n}{2}\right] \left[\frac{2}{k}\right]^{d+n} . \quad (16)$$

Inserting the remaining factors from (14) gives the final result

$$S(\mathbf{k},t) = \frac{1}{\pi} (4\pi)^{(d+n)/2} \frac{\Gamma^2((n+1)/2)\Gamma(d/2)}{\Gamma(n/2)} \frac{\rho_{\rm def}}{k^{d+n}} . \quad (17)$$

We note that this expression is smooth as n passes through the even integers. Equation (17) constitutes the central result of this Rapid Communication. The generality of the result cannot be overemphasized: It is independent of any details of the dynamics, e.g., whether the order parameter is conserved or nonconserved, and holds independently of whether the scaling hypothesis is valid. We note that, as well as providing an exact result against which to test approximate theories, Eq. (17) can also be used to determine the defect density experimentally.

We can compare our result for $C_{\rm sing}$, Eq. (14), with simulation data for $C(\mathbf{r},t)$ presented in Humayun and Bray [14] for the $2d$ Ising model, on a square lattice, quenched to zero temperature. They measure

$$C_{\rm sim} = 1 - 0.525 r/\sqrt{t} , \quad r \ll \sqrt{t} . \quad (18)$$

To compare this result with (14) we need to know the domain-wall density $\rho(t)$, i.e., the length of domain wall per unit area. This can be determined from the residual energy, since for an Ising model all the excess energy is stored in the domain walls. If the bonds have unit strength, the residual energy per spin is $E(t)=2\rho(t)$, since each broken bond costs energy 2. Humayun and Bray measure $E(t)=1.042/\sqrt{t}$ [15], implying $\rho(t)=0.521/\sqrt{t}$. Note, however, that since this definition of ρ gives the number of broken bonds, it measures the length of interface using a Manhattan metric on the square lattice. Equation (14), however, was derived using a continuum description, corresponding to a Euclidean metric. Fortunately, a simple conversion is possible. A piece of wall of Euclidean length unity, at an angle θ to one of the lattice axes, has Manhattan length $(|\cos\theta| + |\sin\theta|)$. Averaging this over θ (assuming isotropy on large scales [14]) gives the ratio of Manhattan to Euclidean lengths as $4/\pi$. Hence the Euclidean wall density is $\rho_E(t) = (\pi/4) \times 0.521/\sqrt{t}$. Substituting this result in (14), with $d=2$ and $n=1$, gives $C_{\rm sing} = -0.521 r/\sqrt{t}$, in good agreement with (18). Simulations on systems with vector order parameters are also underway [16]. Preliminary results indicate good agreement with (17), after correcting for the lattice geometry.

As has been emphasized, the exact result (17) [or, equivalently, (14)] can be used to test existing theories for $C(\mathbf{r},t)$. Here we examine theories of the ordering kinetics of nonconserved fields. To establish the units of time, we will take the dynamics to be governed by the time-dependent Ginzburg-Landau equation $\partial_t \vec{\phi} = \nabla^2 \vec{\phi} - dV(\vec{\phi})/d\vec{\phi}$. The most successful theoretical approaches [17,18,3–6] are based on the introduction of a smooth auxiliary field $\vec{m}(\mathbf{r},t)$ designed to eliminate the rapid spatial variation of $|\vec{\phi}|$ that occurs near topological defects (originally [17], near domain walls in a scalar field). To achieve this, the function $\vec{\phi}(\vec{m})$ is conveniently chosen to mimic the equilibrium defect profile function, so that $\vec{m}$ can be interpreted, near defects, as a coordinate normal to the defect [18,5,6]. In order to make analytical progress, the field $\vec{m}$ is taken to have a Gaussian distribution, an approach taken to its logical conclusion in the work of Mazenko [18] and subsequent extensions [5,6].

In order to compare theoretical predictions with (14) or (17) we need to be able to separately calculate both $C(\mathbf{r},t)$ and the defect density $\rho_{\rm def}$. The latter is given by $\rho_{\rm def} = \langle \delta(\vec{m}) J[\vec{m}] \rangle$, where $J[\vec{m}]$ is the Jacobian of the transformation from the field $\vec{m}$ to the spatial coordinate $\mathbf{r}$, e.g., for a scalar field $J[m] = |\nabla m|$. Since, however, the spatial variation of $\vec{m}$ near a defect is the same for all defects of a given type, it follows that $J[\vec{m}]$, evaluated at a defect, is a (calculable) constant, and can be taken outside the average to give [19] $\rho_{\rm def} = J\langle \delta(\vec{m}) \rangle = JP(0)$, where $P(\vec{m})$ is the probability distribution for $\vec{m}$.

Making now the Gaussian assumption for $\vec{m}$, both $C(\mathbf{r},t)$ and $\rho_{\rm def}$ can be calculated. One finds [5,6] a scaling solution, with growth law $L(t) \sim t^{1/2}$. The two-point correlation function has a short-distance singularity of the form [5,6]

$$C_{\rm sing}^{\rm Gaussian} = \frac{1}{\pi}\frac{\Gamma^2((n+1)/2)\Gamma(-n/2)}{\Gamma(n/2)}\left[\frac{\lambda}{2dt}\right]^{n/2}|\mathbf{r}|^n , \tag{19}$$

while the defect density is [19]

$$\rho_{\rm def} = (\lambda/4\pi t)^{n/2} , \tag{20}$$

and scales as $L(t)^{-n}$, as it should. [For $n=1$, the d appearing in (19) has to be replaced by $(d-1)$ [5,6].] In (19) and (20), λ is a parameter of the Mazenko theory related to two-time correlations [5,6]. In the simpler approach of Bray and Puri [3], it has the value $d/2$. Equation (20) can now be used in (19) to eliminate the explicit time dependence and derive an equation, analogous to (14), connecting $C_{\rm sing}$ to $\rho_{\rm def}$. Comparing the result with (14) we obtain the ratio

$$\frac{C_{\rm sing}^{\rm Gaussian}}{C_{\rm sing}^{\rm exact}} = \frac{\Gamma((d+n)/2)}{\Gamma(d/2)}\left[\frac{2}{d}\right]^{n/2} , \tag{21}$$

from which λ has dropped out. This ratio is, in general, different from unity. It does equal unity for $n=2$, which is probably not significant, and for $d\to\infty$, which probably is: there are other indications [6,20] that these Gaussian theories become exact for $d\to\infty$.

An alternative way of calculating $\rho_{\rm def}$ is to leave the Jacobian $J[\vec{m}]$ inside the average before applying the Gaussian approximation [21]. Then the result cannot be written as simply as (20): Indeed, the calculation has not been performed for general n and d. For the known special cases ($n=1$, all d, and $d\le 3$, $n\le d$) the ratio $C_{\rm sing}^{\rm Gaussian}/C_{\rm sing}^{\rm exact}$ is different from unity, except for $n=1$. For $d\to\infty$, the two ways of calculating $\rho_{\rm def}$ agree for $n=1$. If, as we suspect [20], the Gaussian theories are exact for $d\to\infty$, the two methods should agree for all n in this limit.

We conclude with a discussion of the universal aspects of the result (17). The derivation given above is restricted to $T=0$, in that thermal fluctuations have been ignored. For $T>0$ (but $T<T_c$), extended defects (walls, strings, etc.) will acquire thermal excitations, and at the same time thermal fluctuations will reduce the equilibrium order parameter. After coarse graining beyond the thermal correlation length ξ, however, the system will be effectively at low temperature and the previous results will be recovered for $k\xi \ll 1$ (but $kL \gg 1$). The only modification to (17) is that a factor $M^2(T)$ has to be included, where $M(T)$ is the magnitude of the equilibrium order parameter, reduced from its saturated value of unity by thermal fluctuations. In addition, the defects whose density is measured by $\rho_{\rm def}$ have to be interpreted as average defects, obtained by time averaging over thermal fluctuations.

In summary, exact results have been presented for the tail of the structure factor in systems with topological defects. Our central result, Eq. (17), extends the classic result of Porod to general O(n) models in arbitrary spatial dimension. It provides an exact result against which to test approximate theories, and facilitates experimental determinations of $\rho_{\rm def}$. A natural question to ask is whether the $k^{-(d+n)}$ tail in $S(\mathbf{k},t)$ survives in systems *without* topological defects. Recent simulation studies [22] of phase ordering in systems with $n>d+1$ suggest a decay for $S(\mathbf{k},t)$ which is faster than any power law in k. While analytic solutions for the tail in the defectless case of $n>d+1$, and in the case $n=d+1$, which admits textures, are clearly desirable, the results presented above for $n\le d$ have the greatest relevance for the analysis of experimental data.

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