Structure factor tail for the ordering kinetics of nonconserved systems without topological defects

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Using a cell-dynamic system simulation scheme, we investigate the phase-ordering dynamics of nonconserved $O(n)$ models without topological defects, i.e., for $n>d+1$ where d is the spatial dimensionality. In particular, we consider zero-temperature quenches for $d=2$, $n=4,5$ and for $d=1$, $n=3,4,5$. We find, in agreement with previous simulations using fixed-length spins, that dynamical scaling is obtained, with characteristic length $L(t)=t^{1/2}$. We show that the asymptotic behavior of the structure-factor scaling function $g(q)$ is well fitted by the stretched exponential form $g(q)\sim\exp(-bq^{\delta})$, with an exponent δ that appears to depend on both n and d. An analytical treatment of an approximate large-n equation for the pair correlation function yields $g(q)\sim q^{-(d-1)/2}\exp(-bq)$, with $b\sim(\ln n)^{1/2}$ for large n, in agreement with recent simulations of the same equation. [S1063-651X(96)07205-4]

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I. INTRODUCTION

The phase-ordering dynamics of systems quenched from a high-temperature disordered state into an ordered state is a problem of great relevance in the description of out-of-equilibrium pattern formation [1]. One well established property is the onset of dynamic scaling, where the late-time behavior of the order-parameter correlation functions is described by scaling forms with a single time-dependent length scale $L(t)$. Thus the real-space correlation function is found to have the scaling form

$$C(r,t)=f(r/L(t)), \tag{1.1}$$

while its Fourier transform, the structure factor, has the corresponding scaling form

$$S(k,t)=[L(t)]^{d}g(kL(t)). \tag{1.2}$$

Conventional experimental systems such as binary alloys and binary liquids are described by a scalar order parameter. Recently, however, there has been much interest in systems with more complicated order parameters such as n-component vectors [the $O(n)$ model] [1–15] and traceless symmetric tensors (nematic liquid crystals) [16]. In this paper we restrict our discussion to the $O(n)$ model.

Much numerical and theoretical effort has been devoted to understanding the basic properties of systems that can support singular topological defects, i.e., systems with $n\leqslant d$. The presence of such defects leads to a generalization of the usual Porod law for the large-q tail of the structure-factor scaling function $g(q)$, namely, $g(q)\sim q^{-(d+n)}$ for $q\gg 1$ [6]. This result is geometrical in origin, and is independent of whether or not the order parameter is conserved by the dynamics [7].

Very recently, the cases $n=d+1$, for which nonsingular topological textures occur, have been studied numerically (for $d=2$) and analytically (for $d=1$). Rutenberg and Bray [8] found that the $d=1$ XY model ($n=2$) exhibits a scaling violation due to the existence of *two* relevant length scales: the phase coherence length and phase winding length. On the other hand, the two-dimensional Heisenberg model ($n=3$) with nonconserved dynamics also violates dynamic scaling due, it appears, to the existence of as many as three separate length scales, related to individual texture size, the typical separation between textures, and the typical distance between textures of opposite charge [9]. These texture systems are, perhaps, the most complex of the phase ordering systems.

By contrast, systems without topological defects ($n>d+1$) seem relatively straightforward. There is good evidence for the simple scaling behavior described by (1.1) and (1.2), with characteristic scale $L(t)\sim t^{1/2}$ for nonconserved dynamics. The energy scaling approach of Bray and Rutenberg [17] shows that, provided scaling holds, $L(t)\sim t^{1/2}$ is indeed correct for $n>d+1$ systems with nonconserved dynamics, and gives $L(t)\sim t^{1/4}$ for conserved dynamics, again nicely consistent with simulation results [10] and the renormalization group result of Bray [18].

Much less is known, however, about the form of the structure-factor tail for $n>d+1$. The recent simulations of Rao and Chakrabarty (RC) [10], with conserved dynamics, for the cases $d=1$, $n=3$ and $d=2$, $n=4$ show ''squeezed exponential'' behavior [i.e., $g(q)\sim\exp(-bq^{\delta})$ with $\delta>1$]. In this paper we concentrate on systems with $n>d+1$ and nonconserved dynamics. We consider the cases $d=2$, $n=4,5$ and $d=1$, $n=3,4,5$. In each case we confirm the expected $t^{1/2}$ growth, and find ''stretched exponential'' behavior [i.e., $g(q)\sim\exp(-bq^{\delta})$ with $\delta\leqslant 1$] for the tail of the structure factor, with an exponent δ that appears to depend on n and d.

In an attempt to understand the origin of this tail behavior, we present an analytical approach based on an approximate equation due to Bray and Humayun (BH) [12], which is itself based on the ''Gaussian auxiliary field'' (GAF) method [14] that describes rather well the form of the structure factor for nonconserved systems with singular defects ($n\leqslant d$). For those systems, this method reproduces, in particular, the gen-

eralized Porod tail. For $n>d+1$, the physical basis of the method is less clear. However, the simple truncation of the equation at leading order in $1/n$, proposed by BH in another context [12], leads to an exponential decay of $g(q)$, modified by a power-law prefactor for $d>1$. It is noteworthy that the asymptotic behavior is nonanalytic in $1/n$: for n strictly infinite, the Gaussian form $g(q)\sim\exp(-2q^2)$ is obtained. The exponential asymptotics of the BH equation were noted in recent numerical studies by Castellano and Zannetti [13].

Using a ''hard-spin'' model Newman, Bray, and Moore [5] studied numerically the dynamics of one-dimensional systems without defects for $n=3,4$, and 5. Measuring only the real-space correlations, they found that dynamic scaling is obeyed with characteristic length $L(t)=t^{1/2}$. Moreover, they found the real-space correlation function was very well fitted by a Gaussian form, which is the exact result in the limit $n\to\infty$. The Fourier space analysis presented here, revealing stretched exponential tails, shows that the good Gaussian fits achieved in real space are misleading.

Our main results can be summarized as follows. (i) For all our models the characteristic length scale required to collapse the data for the real-space correlation function and structure factor is $L(t)=t^{1/2}$, in agreement with theoretical predictions [17]. (ii) The asymptotic behavior of the structure factor is well described by a stretched exponential of the form $g(q)\sim\exp(-bq^{\delta})$, where the exponent δ apparently depends on both n and d and seems to be different from the value obtained for the corresponding system with conserved dynamics [10]. (iii) An analytical treatment of the approximate BH equation, expected to be valid at large (but finite) n, gives a simple exponential modified by a power, $g(q)\sim q^{-(d-1)/2}\exp(-bq)$, with the *same* asymptotic form for conserved dynamics.

The rest of this paper is organized as follows. In the next section, we introduce the cell-dynamic system (CDS) model based on the time-dependent Ginzburg-Landau (TDGL) equation for a zero-temperature quench, and we describe the corresponding numerical procedure employed in the simulation. Section III presents simulation results for a vector order parameter with $n=4$ and $n=5$ components in one and two dimensions and the one-dimensional $O(3)$ model. For the $d=2$ systems, we also present data for the real-space correlation function to demonstrate the dynamic scaling behavior. We then discuss the procedure used to obtain the asymptotic functional form of the structure factor tail. Next we compare the data to the results of the approximate analytic theory. Finally we make some concluding comments on our results and a give a brief summary.

II. MODEL AND SIMULATIONS

The dynamic evolution of a nonconserved vector order parameter (model A) with n components $\vec{\phi}=(\phi_1,\phi_2,\ldots,\phi_n)$, for a zero-temperature quench, is described by a purely dissipative process defined in term of the following TDGL equation:

$$\frac{\partial\vec{\phi}(\mathbf{x},t)}{\partial t}=-\Gamma\frac{\delta F(\vec{\phi}(\mathbf{x},t))}{\delta\vec{\phi}(\mathbf{x},t)}, \tag{2.1}$$

with Γ a kinetic coefficient that we will set equal to unity, and F the free energy functional that generates the thermodynamic force,

$$F[\vec{\phi}(\mathbf{x},t)]=\int d^d\mathbf{x}\left[\frac{1}{2}[\nabla\vec{\phi}(\mathbf{x},t)]^2+V(\vec{\phi}(\mathbf{x},t))\right], \tag{2.2}$$

with the potential defined as

$$V(\vec{\phi}(\mathbf{x},t))=\tfrac{1}{4}[1-\vec{\phi}^2(\mathbf{x},t)]^2, \tag{2.3}$$

where $\vec{\phi}^2=\Sigma_{i=1}^{n}\phi_i^2(\mathbf{x},t)$. The ground states, or fixed points of the dynamics, are determined by the condition $\vec{\phi}^2=1$, which defines a degenerate manifold of states connected by rotations. In the internal space of the order parameter, this manifold is the surface of an n-dimensional sphere. At late times the order parameter is saturated in length (i.e., lies on the ground state manifold everywhere). Then the dynamics is driven by the decrease of the free energy associated with the term $(\nabla\vec{\phi})^2$ in (2.2), through a reduction in the magnitude of the spatial gradients.

We can construct an explicit numerical scheme for the simulation based on a computationally efficient algorithm, namely, the CDS [19], which updates the order parameter according to the rule

$$\vec{\phi}(\mathbf{x},t+1)=H(\vec{\phi}(\mathbf{x},t))+\tau D\left[\frac{1}{z}\sum_{\mathbf{x}'}\vec{\phi}(\mathbf{x}',t)-\vec{\phi}(\mathbf{x},t)\right], \tag{2.4}$$

with

$$H(\vec{\phi}(\mathbf{x},t))=\vec{\phi}(\mathbf{x},t)+\tau\vec{\phi}(\mathbf{x},t)[1-(\vec{\phi}(\mathbf{x},t)^2)], \tag{2.5}$$

where z is the number of nearest neighbors and τ and D are parameters that we choose to be $\tau=0.2$ and $D=0.5$ in our simulations.

The above numerical procedure is identical to that used by Toyoki [15], differing only in the values of the parameters τ and D. The CDS is a Euler-like algorithm and for convenience in our analysis of the results we use a unit of time equal to the update time step τ. It should be noted (see Figs. 1 and 3) that the scaling regime is reached very quickly in these systems without defects, and very long runs are not necessary.

The two-dimensional systems consist of a square lattice of size 256×256 with periodic boundary conditions. The physical quantities are calculated as averages over 20 independent distributions of initial conditions. The one-dimensional systems have $L=16\,384$ sites (with periodic boundary conditions) and we average 100 independent runs. The initial conditions for the order parameter components $\vec{\phi}_i$ were randomly chosen from a uniform distribution with support on the interval $(-0.1,0.1)$.

A quantity of interest that is computed during the course of the numerical simulation in the two-dimensional models is the two-point real-space correlation function

$$C(\mathbf{r},t)=\langle\vec{\phi}(\mathbf{x},t)\cdot\vec{\phi}(\mathbf{x}+\mathbf{r},t)\rangle, \tag{2.6}$$

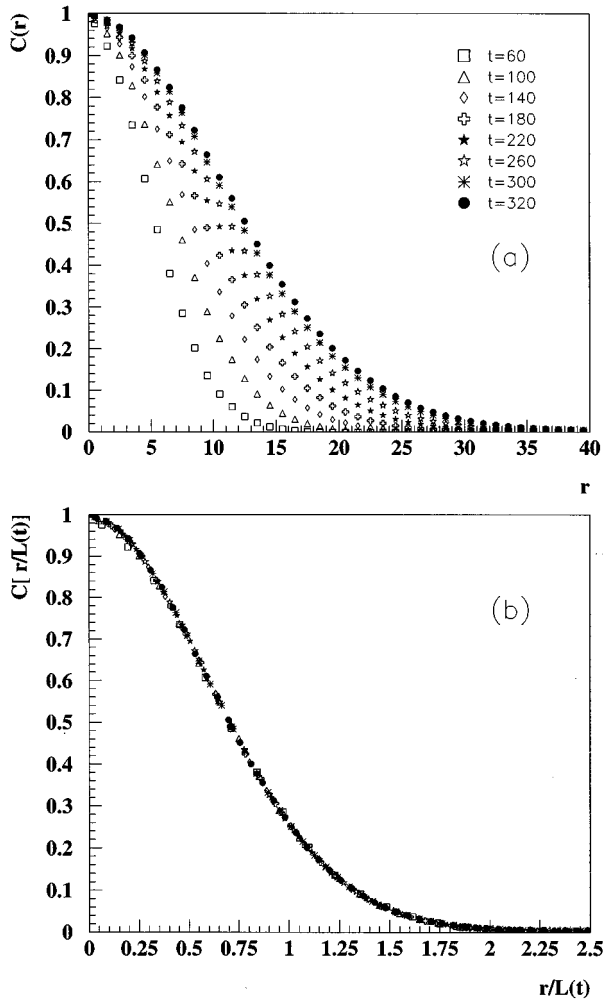

FIG. 1. (a) Real-space correlation function $C(r)$ for a two-dimensional system with $n=4$ components as a function of distance r for several times t. The data were obtained from lattices of size 256×256, averaged over 20 different initial conditions. (b) Demonstration of dynamic scaling, $C(r,t)=f(r/L(t))$, with $L(t)=t^{1/2}$.

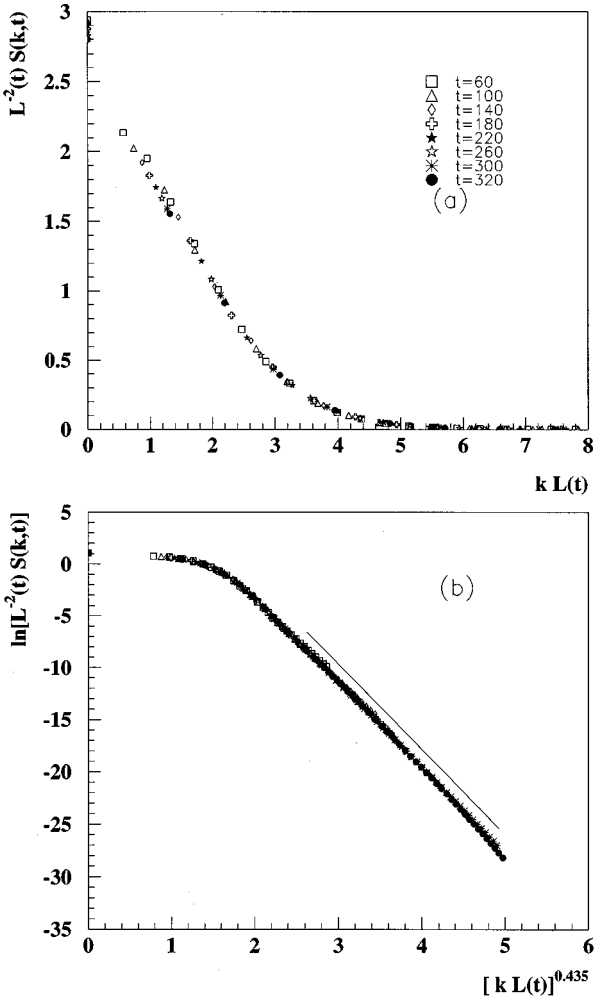

FIG. 2. (a) Scaling structure factor $g(q)=[L(t)]^{-2}S(k,t)$ as a function of scaled momentum $q=kL(t)$ for a two-dimensional system with $n=4$ components for lattices of size 256×256 (averaged over 20 different initial conditions). (b) Demonstration of the stretched exponential behavior, plotting $\ln g(q)$ against q^{δ} with $\delta=0.435$. The line is included as a guide to the eye.

where $\langle\ \rangle$ stands for the average over the set of independent initial conditions (or ''runs''). A spherical average over all possible distances $r=|\mathbf{r}|$ is performed to find the isotropic real-space correlation $C(r,t)$. The other function of interest, calculated for all the models, is the structure factor

$$S(\mathbf{k},t)=\langle \vec{\phi}(\mathbf{k},t)\cdot\vec{\phi}(-\mathbf{k},t)\rangle. \tag{2.7}$$

We also make a spherical average over all possible values of $\mathbf{k}$ with given $k=|\mathbf{k}|$.

In the calculation of these quantities at each time, the data are ''hardened'' by replacing the order parameter at each point by a unit vector in the same direction (the fixed point of the CDS iteration being a vector of unit length). This procedure accelerates the entry into the dynamic scaling regime, and helps us to elucidate the proper nature of the asymptotic tail in the structure factor.

III. RESULTS

Dynamic scaling is observed for all the models studied. The scaling regime is reached at quite early times, in agreement with previous studies. We show that dynamic scaling holds in the two-dimensional systems ($n=4,5$), using the characteristic length $L(t)=t^{1/2}$ deduced from theoretical considerations [17]. This agrees with earlier simulations of Bray and Humayun using ''hard-spin'' dynamics [3].

Figure 1(a) presents a plot for $d=2$, $n=4$ of the correlation function (1.1) as a function of distance r for several times, while in Fig. 1(b) we show the collapsed dynamic scaling function when the analysis is made using the scaling variable $x=r/L(t)$. As can be seen from the figure, the scaling function $f(x)$ is a monotonically decreasing function with the generic featureless shape that is characteristic of nonconserved $O(n)$ models.

It is of some interest to investigate the small-x behavior of the real-space scaling function $f(x)$. In systems with $n\leqslant d$, the existence of singular topological defects leads to a

TABLE I. Parameters determined from fitting of the simulation results for the two-dimensional systems: the small-x solution ($x<0.5$) in the scaling function with the form $f(x)=1-\alpha x^2+\beta x^4$ and the asymptotic analysis of scaling structure factor in term of the stretched exponential $g(q)\sim\exp(-bq^{\delta})$.

	Small x		Tail	
n	α	β	δ	b
4	1.5326	1.3916	0.435	8.19
5	1.3040	0.8417	0.613	4.39

nonanalytic term of the form $|x|^n$ (with an additional ln$x$ factor for even n), which leads to the $k^{-(d+n)}$ Porod tail in Fourier space [6,7]. In the present case, where $n>d$, we expect no such short-distance singularities. Therefore, we consider an expansion of the form $f(x)=1-\alpha x^2+\beta x^4\cdots$. In Table I we present the parameters α and β determined from the simulations in the range $x<0.5$. The ratio $r=\beta/\alpha^2$ should be a universal number for given n and d. It will be seen from Table I that this ratio has the value $r\simeq 0.59$ for $n=4$, different from the value 1/2 obtained for a Gaussian function, which is the exact result for the limit $n\to\infty$. For $n=5$, Table I gives $r\simeq 0.49$, already consistent with the large-n result. However, in the absence of any short-distance singularity, the small-x behavior provides no useful information on the nature of the tail in the structure factor. Consequently, it is more convenient to investigate directly the simulation results of the structure factor and extract from them the asymptotic behavior. We shall see that the behavior in Fourier space is clearly non-Gaussian, even for $n=5$.

As expected, given the absence of topological defects, the results indicate (Fig. 2) that the decay of the structure factor is clearly faster than a power law, in contrast to the interpretation of his own similar results by Toyoki [15]. In order to demonstrate that the tail is well described by the stretched exponential form

$$g(q)\sim A\exp(-bq^{\delta}), \tag{3.1}$$

where $q=kL(t)$ is the scaling variable in momentum space, we attempt to find the corresponding power δ in the exponential by plotting ln$g$ versus q^{δ} and adjusting the value of δ until the best linear behavior is obtained in the regime $q>1$. During the fitting procedure the other two parameters of the fit, A and b, are readily determined. The criteria used for the optimum fitting is based on the Pearson correlation coefficient (PCC), which measures the strength of the linear relation among two variables and varies between -1 (perfect negative linear relation) and $+1$ (perfect positive linear relationship). We proceed as follows: first, we choose an exponent δ and then perform linear regression; next we change δ until the PCC reaches its maximum value. The regression coefficients are calculated using the values of the scaling structure function at the last two times in the simulation. The optimum values for system with $n=4$ components are $\delta=0.435$ with a Pearson coefficient of -0.999998. The other two parameters are ln$A=13.21$ and $b=8.19$. This result is presented in the Fig. 2(b).

We turn now to the description of the case $n=5$, following a similar analysis to the $n=4$ model. Figure 3(a) shows

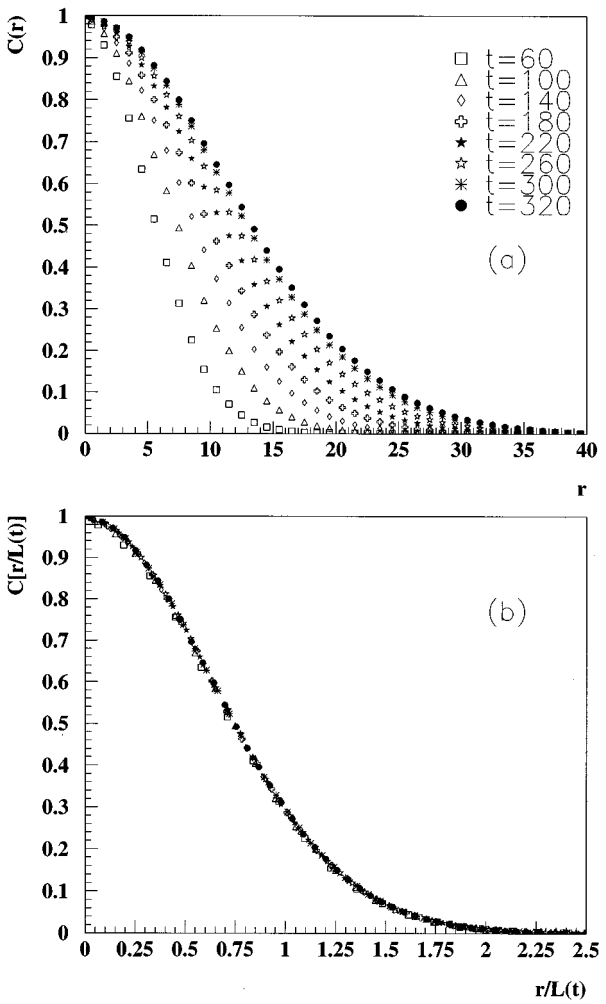

FIG. 3. Same as Fig. 1 but for the $n=5$ model.

the correlation function as a function of distance for different times. In this model the collapse is also achieved using the characteristic length $L(t)=t^{1/2}$, as can be observed in Fig. 3(b). Therefore, both models are consistent with dynamical exponent $z=2$. The corresponding scaling plot for the structure factor is shown in Fig. 4(a). A more important effect is observed in the structure factor tail, because in this case it also has a stretched exponential but with an apparently larger exponent. Following an analysis similar to that used for $n=4$, we find that the value of the best fit value of the exponent is $\delta=0.613$, and the corresponding PCC in the regression is -0.999998. The other two parameters are ln$A=7.57$ and $b=4.39$. In Fig. 4(b) we plot ln$g$ against q^{δ} and the linear behavior is seen clearly.

Comparison between the real-space correlation functions of the $n=4$ and $n=5$ models shows that the scaling functions are very similar; the main difference is that the scaling function decreases slightly more slowly for $n=5$ than for $n=4$. This is reflected in the parameters of the fitting function for the small-x range: the amplitudes α and β tend to decrease as n increases (Table I).

We turn to a discussion of the simulation results for one-dimensional systems. We shall describe the relevant behavior in Fourier space. Real-space data have been presented in [5]. Our results show that in one-dimensional systems the

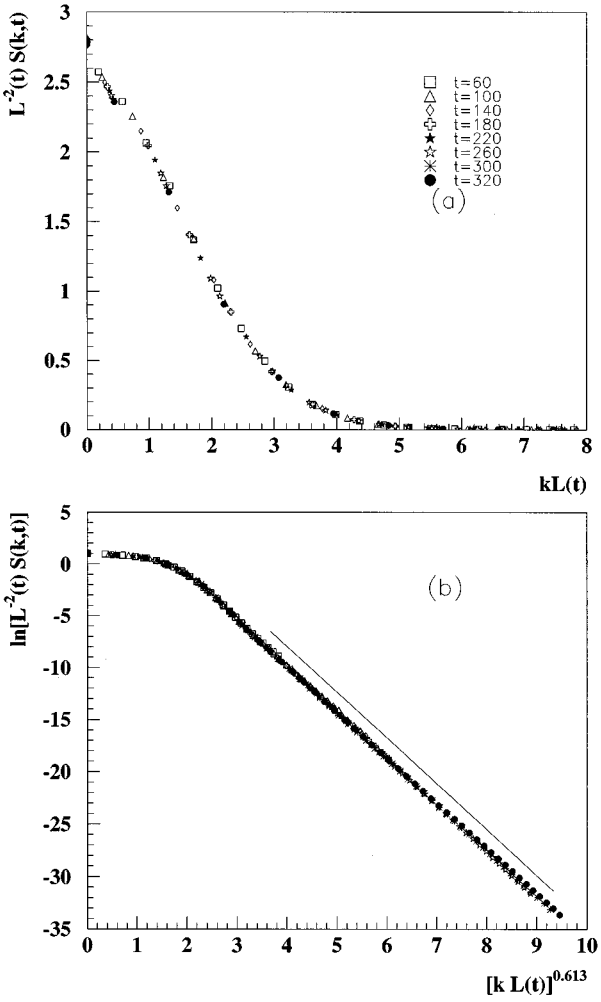

FIG. 4. (a) Same as Fig. 2 but for the $n=5$ model. (b) The power $\delta=0.613$ was found to give the best linear relation between $\ln g(q)$ and q^{δ}.

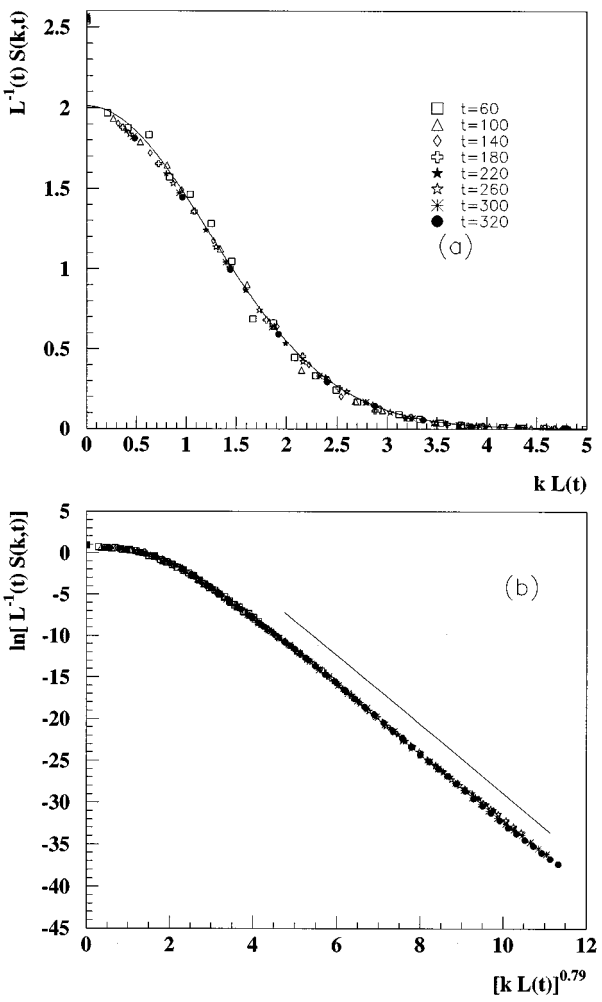

FIG. 5. (a) Scaling structure factor $g(q)=[L(t)]^{-1}S(k,t)$ as a function of scaled momentum $q=kL(t)$ for a one-dimensional Heisenberg model [$O(3)$ model] for lattices of size 16 384 (averaged over 100 different initial conditions). Continuous curve: result of the approximate analytical treatment described in the text. (b) Demonstration of the stretched exponential behavior, plotting $\ln g(q)$ against q^{δ} with $\delta=0.79$. The line is a guide to the eye.

asymptotic behavior of the structure factor also has a stretched exponential form, but the fitted exponents δ are larger than those of the corresponding two-dimensional models, and close to unity for $n=4$ and 5.

In Fig. 5(a), we present the simulation results for the scaling function $g(q)$ of the structure factor for the one-dimensional Heisenberg Model ($n=3$). The continuous curve is the result of the analytical approach described in Sec. IV. The analysis of the asymptotic behavior gives an exponent $\delta=0.79$ for the stretched exponential. Fig. 5(b) shows the curve of $\ln[g(q)]$ versus q^{δ}, where the linear behavior is clearly observed. Similarly, we present the corresponding plots for the $n=4$ model in Fig. 6, where the measured exponent is now $\delta=0.98$, while for $n=5$ we obtain $\delta=1.02$ as is shown in Fig. 7. The values of δ for the last two models are so close that in practice it is difficult to distinguish between them. They are also close to the value unity obtained from the approximate large-n equation discussed in the following section.

It is clear from the results for the one-dimensional models that the scaling function in real space is not a Gaussian function, despite the good real-space fits to this form obtained in [5]. Moreover, the (effective) exponents δ for the $n=4,5$ models are bigger than for the corresponding models in two dimensions. Therefore, we have evidence that the exponent δ increases with n, while it seems to decrease with d. Note that the Gaussian result obtained for $n=\infty$ corresponds to $\delta=2$, so the results presented here for the structure-factor tail are actually quite far from that limit. The analytical treatment presented in the next section gives some indication of why this might be expected. In particular, it suggests that the structure factor is dominated by a simple exponential for $q\to\infty$ at fixed large n, while the familiar Gaussian form is recovered as $n\to\infty$ at fixed q.

We conclude this section by discussing briefly some alternative fitting forms for the structure factor tail. First, however, we note that the stretched exponential form (3.1) describes the tail well over at least 10 decades of $S(k)$ in all cases. Of course, this represents a much smaller dynamic range (1 to $1\frac{1}{2}$ decades) in the scaling variable $q=kL(t)$. Motivated by the analytical result [Eq. (4.7) below] of the approximate large-n theory, other fitting forms were tried for

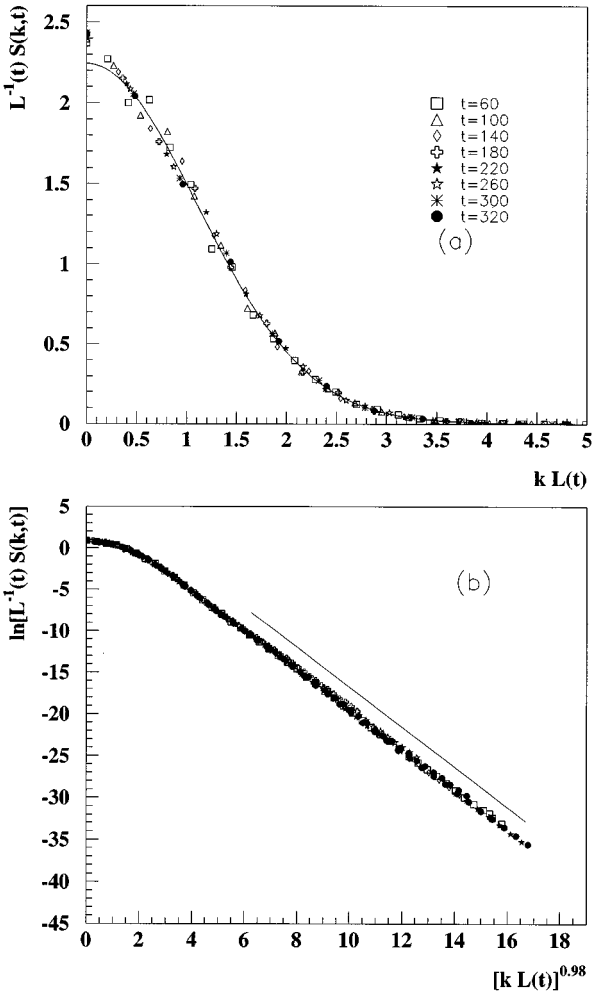

FIG. 6. (a) Same as Fig. 5, but for the $n=4$ model. (b) The power $\delta=0.98$ is found for this model to give the best linear relation between $\ln g(q)$ and q^{δ}.

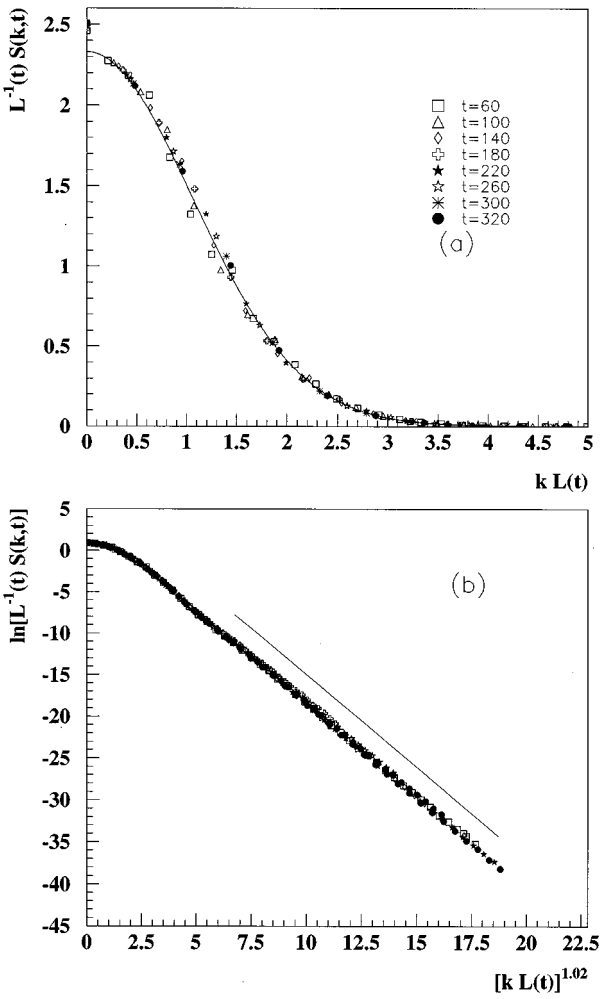

FIG. 7. (a) Same as Fig. 5 but for the $n=5$ model. (b) Same as Fig. 5(b), but with $\delta=1.02$.

$d=2$ (the agreement with the large-n theory already being good for $n=4$ and 5 in $d=1$). A direct fit of (4.7) does not work well for $d=2$. Allowing for a general power-law prefactor, $g(q)=Aq^{-x}\exp(-bq)$, gives a reasonable fit, but with very large values for x — 5.6 for $n=4$ and 6.7 for $n=5$. Fixing $x=1/2$, but allowing for a general stretched exponent δ again gives a reasonable fit (with $\delta\simeq 0.68$ for $n=4$ and 0.70 for $n=5$), but over a significantly reduced range of q. For these reasons we prefer the unmodified stretched exponential (3.1) as giving the simplest and most convincing description of the large-q data, at least for these small values of n in $d=2$. Of course, it is quite possible that the form (4.7) will fit the data well at larger values of n.

IV. ANALYTICAL TREATMENT

In an attempt to gain some analytical insight into the structure factor asymptotics, we start from an approximate equation of motion for the pair correlation function derived using the Gaussian auxiliary field approach pioneered by Mazenko [20]. We then make, for reasons that will become clear, the further simplification of retaining only the leading nonlinearity as $n\to\infty$. The resulting equation is then finally used to extract the asymptotics of $g(q)$.

The GAF method for vector fields has been discussed in some detail elsewhere. We refer the reader to the original papers [14] and a recent review [1] for a full exposition. The essence of the method is a mapping from the original field variable $\vec{\phi}$ to an ''auxiliary field'' $\vec{m}$. The function $\vec{\phi}(\vec{m})$ satisfies the equation $(1/2)\Sigma_{i=1}^{n}\partial^2\vec{\phi}/\partial_{m_i}^2=\partial V/\partial\vec{\phi}$, where $V(\vec{\phi})$ is the potential in the Ginzburg-Landau function (4). With the boundary conditions $\vec{\phi}(0)=0$, and $\vec{\phi}(\vec{m})\to\vec{m}/|\vec{m}|$ for $|\vec{m}|\to\infty$, this equation for $\vec{\phi}(\vec{m})$ represents the equilibrium profile function for a spherically symmetric topological defect, with $|\vec{m}|$ representing distance from the defect.

The (uncontrolled) approximation that $\vec{m}$ is a Gaussian field, and the imposition of the scaling form (1), leads eventually to the self-consistent equation [1,14]

$$f''+\left(\frac{d-1}{4}+\frac{x}{4}\right)f'+\frac{\lambda}{2}\gamma\frac{dC}{d\gamma}=0 \tag{4.1}$$

for the scaling function $f(x)$, where primes indicate derivatives. In (4.1) γ is the normalized correlator of the auxiliary

field, $\gamma=\langle\vec{m}(1)\cdot\vec{m}(2)\rangle/[\langle\vec{m}^2(1)\rangle\langle\vec{m}^2(2)\rangle]^{1/2}$, where 1 and 2 represent the space-time points $\mathbf{x}_1,t$ and $\mathbf{x}_2,t$, and the function $C(\gamma)$ is given by

$$C(\gamma)=\frac{n\gamma}{2\pi}\left[B\left(\frac{n+1}{2},\frac{1}{2}\right)\right]^2 F\left(\frac{1}{2},\frac{1}{2};\frac{n+2}{2};\gamma^2\right), \quad (4.2)$$

where $B(x,y)$ is the β function, and $F(a,b;c;z)$ the hypergeometric function. The constant λ in (4.1) has to be adjusted so that $f(x)$ vanishes sufficiently fast at infinity [14].

As should be clear from the above discussion, (4.1) only really makes sense for $n\leqslant d$, based as it is on the presence of singular topological objects whose positions are defined by the zeros of the field $\vec{\phi}$ or, equivalently, by the zeros of $\vec{m}$. Indeed, the function $C(\gamma)$ has a built-in structure that generates the Porod tail associated with such defects. Specifically, in the short-distance limit, where $\gamma\to 1$, the hypergeometric function in (4.2) has a singular contribution of order $(1-\gamma^2)^{n/2}$ (with a logarithmic correction for even n). Since $1-\gamma^2\sim x^2$ for small scaling variable x, this singular term is of order x^n (again, with a logarithm for even n), leading to the power-law tail $g(q)\sim q^{-(d+n)}$ in Fourier space. Within the GAF approach, this tail is obtained for *all* n and d. For $n>d+1$, however, neither singular topological objects nor nonsingular topological textures exist, so the GAF result is qualitatively incorrect. Indeed, this is to be expected since the GAF approach is specifically designed to build in the defect structure.

So what should one do when there are no defects? We have seen that the usual GAF approach always gives a Porod tail, for any n and d: this is unphysical for $n>d+1$, since the tail is a consequence of the presence of topological defects. One way around this impasse is to artificially approximate the full GAF equation (4.1) by the form valid for $n\to\infty$. In this limit $\gamma dC/d\gamma=f+f^3/n+O(1/n^2)$, and (4.1) becomes, correct to $O(1/n)$,

$$f''+\left(\frac{d-1}{4}+\frac{x}{4}\right)f'+\frac{\lambda}{2}\left(f+\frac{1}{n}f^3\right)=0. \quad (4.3)$$

This step, admittedly *ad hoc*, has the desired effect of eliminating the unwanted (for $n>d+1$) short-distance singularity in $f(x)$. Equation (4.3) is the nonconserved version of the equation introduced by BH to study the crossover from multiscaling to simple scaling in the asymptotic dynamics of a *conserved* vector field at large but fixed n [12]. Both conserved and nonconserved versions have recently been studied numerically [13].

To extract analytically the large-q behavior, we perform a (d-dimensional) Fourier transform of (4.3). The resulting equation for $g(q)\equiv\int d^dx f(x)\exp(i\mathbf{q}\cdot\mathbf{x})$ is

$$\left(\frac{d}{4}+q^2\right)g(q)+\frac{q}{4}g'(q)=\frac{\lambda}{2}[g(q)+B(q)], \quad (4.4)$$

where

$$B(q)=\frac{1}{n}\int d^dx f^3(x)\exp(i\mathbf{q}\cdot\mathbf{x}). \quad (4.5)$$

If we assume an asymptotic form $g(q)\sim q^\nu\exp(-bq^\delta)$, with $\delta<2$, then (4.4) gives

$$B(q)\to\frac{2q^2}{\lambda}g(q), \quad q\to\infty. \quad (4.6)$$

In the Appendix, we show that consistency with (4.6) requires $\delta=1$ and $\nu=(1-d)/2$, i.e.,

$$g(q)\to Aq^{(1-d)/2}\exp(-bq), \quad q\to\infty. \quad (4.7)$$

In real space this implies that the function $f(z)$ has simple poles in the complex z plane at $z=\pm ib$. The value of b is not determined by this argument; instead one can derive (see Appendix) the relationship

$$A^2=(16\pi^2 n/\lambda)(2\pi b)^{d-1} \quad (4.8)$$

between b and the prefactor A in the asymptotic form (4.7). The existence of these simple poles in real space also follows directly from the real-space equation (4.3). If one assumes a singularity of the form $(z-z_0)^{-\gamma}$, with $\gamma>0$, then balancing the dominant terms f'' and $\lambda f^3/2n$ gives immediately $\gamma=1$, i.e., a simple pole. The position z_0 is not determined, but the residue C of the pole is given by $C=\mp i(4n/\lambda)^{1/2}$, where the two values correspond to the poles $z_0=\pm ib$. Using this result for C, one can readily recover (4.8) by contour methods, e.g., for $d=1$ one has

$$g(q)=\int_{-\infty}^{+\infty}dx f(x)\exp(iqx)$$
$$\to 2\pi(4n/\lambda)^{1/2}\exp(-bq), \quad q\to\infty, \quad (4.9)$$

where the second line, equivalent to (4.8) for $d=1$, was obtained by closing the contour in the upper half plane.

The approach outlined above gives the relation (4.8) between A and b, but does not determine b explicitly. We now give a heuristic argument that $b\sim(\ln n)^{1/2}$ for large n. First we make an observation concerning the value of λ. Equation (4.4) with $q=0$ gives

$$\lambda=\frac{d}{2}\frac{g(0)}{g(0)+B(0)}$$
$$=\frac{d}{2}\left[1+\frac{1}{n}\int d^dx f^3(x)\Big/\int d^dx f(x)\right]^{-1}. \quad (4.10)$$

In particular, $\lambda=d/2$ for $n=\infty$. For $n=\infty$, therefore, (4.4) becomes $q^2g(q)+(q/4)g'(q)=0$, with solution $g(q)=(8\pi)^{d/2}\exp(-2q^2)$ [the prefactor being fixed by the condition $f(0)=1$]. For n large but finite, on the other hand, we have seen that the asymptotic form is $g(q)\sim\exp(-bq)$. The crossover between these two forms presumably occurs at some $q=q^*(n)$, with $g(q)\sim\exp(-2q^2)$ for $1\ll q\ll q^*$, and $g(q)\sim\exp(-bq)$ for $q\gg q^*$. Matching these two forms at $q=q^*$ gives $q^*\sim b$. Next we evaluate $B(q)$ in the region $q\ll q^*$. Here $q(q)\simeq(8\pi)^{d/2}\exp(-2q^2)$, so $f(x)\simeq\exp(-x^2/8)$, giving $B(q)\sim(1/n)\exp(-2q^2/3)$. However, this decays more slowly with q than the other terms in (4.4), which fall off as $\exp(-2q^2)$. So the term involving $B(q)$ (evaluated for $q\ll q^*$) becomes comparable with the

other terms when $(1/n)\exp(-2q^2/3) \sim \exp(-2q^2)$, i.e., when $q \sim (\ln n)^{1/2}$. This suggests $q^* \sim (\ln n)^{1/2}$, and therefore $b \sim (\ln n)^{1/2}$. The numerical data of Castellano and Zannetti [13] certainly show that b increases extremely slowly with n.

To compare this approximate theory with our simulation data, we have solved (4.1) numerically for $d=1$, $n=3,4,5$, using the procedure described in [14]. The Fourier transform was then taken numerically, and the ''best fit by eye'' to the structure-factor data was obtained by adjusting the time scale in the theoretical curves, giving the results shown by the continuous curves in Figs. 5(a), 6(a), and 7(a). The corresponding log-linear plots, which reveal the large-q behavior more clearly, are shown in Figs. 8(a)–(c). As might be expected, Eq. (4.1) [or its Fourier transform (4.4)] does not describe the data quantitatively over the whole range of $q=kL(t)$, but it does give a qualitatively correct description. There is an early parabolic region, corresponding to a Gaussian form for $g(q)$, which then gives way to a slower decay that, at least for $n=4$ and 5, is consistent with the simple exponential form predicted by (4.4) but with a different coefficient b in the exponent. Given that the theory is, at best, a large-n theory we regard these results as encouraging. The $n=3$ data, however, and the $d=2$ data, do not seem to fit a simple exponential, at least for the range of q that we have been able to explore. (This is of course implicit in the values $\delta<1$ obtained for these systems from Figs. 2, 4, and 5.) It may well be that considerably larger values of n are needed in $d=2$ than in $d=1$ for the large-n asymptotics to become apparent.

The above derivation of an exponential tail was specific to nonconserved fields. What can we say for conserved fields? The fundamental equation of motion for this case is obtained from the TDGL equation (2.1) by the replacement $\Gamma \to -\Gamma\nabla^2$. Applying the GAF method to this equation, imposing the scaling form (1.1) [but with $L(t)=t^{1/4}$ for conserved fields], and taking the Fourier transform, leads to [12]

$$\left(\frac{d}{8}+q^4\right)g(q)+\frac{q}{8}g'(q)=\frac{\lambda}{2}q^2[g(q)+B(q)], \tag{4.11}$$

instead of (4.4). [The definition (4.5) of $B(q)$ differs by a constant from that used in [12], where λ was written as $2q_m^2$, q_m being the position of the maximum of $g(q)$ for large n.] Assuming the asymptotic form $q(q) \sim q^{\nu}\exp(-bq^{\delta})$ for $q \to \infty$, (4.11) gives (4.6) once more, provided $\delta<4$. Then our previous arguments apply, and the asymptotic form (4.7), with A and b related by (4.8), are recovered. This approach therefore predicts that the structure factors for conserved and nonconserved systems will have the *same* asymptotic forms, at least within the context of the BH truncation. The same conclusion was drawn from recent numerical solutions of the BH equation [13].

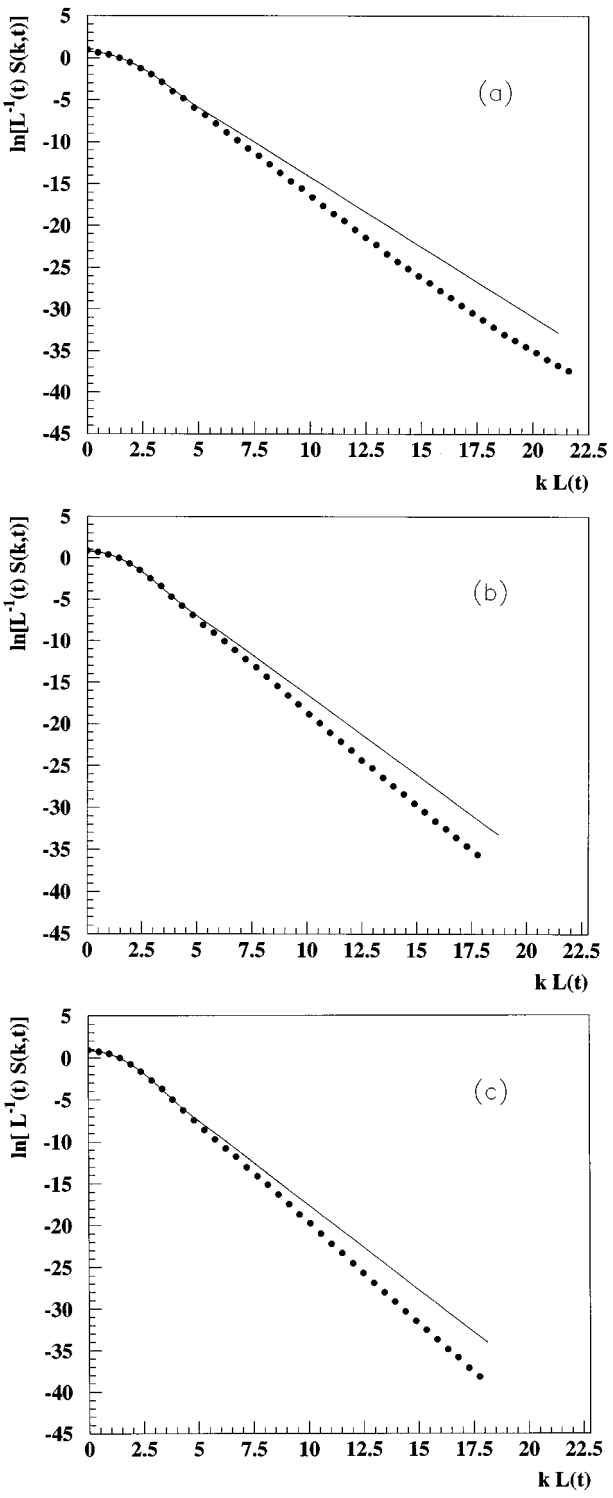

FIG. 8. Log-linear plot of the scaled structure factor against scaled momentum for the one-dimensional systems: (a) $n=3$, (b) $n=4$, (c) $n=5$. In each case the continuous curve is the result of the approximate theory of Sec. IV.

V. CONCLUSION

In summary, we have studied the dynamics of phase ordering for models without topological defects in one and two dimensions. We find that scaling is achieved with the growth law $L(t)=t^{1/2}$. The tail in the structure factor is well fitted by a stretched exponential form. For the two-dimensional systems, Table I summarizes the relevant parameters describing the fits in real and Fourier space. In contrast to systems with singular defects ($n \leqslant d$), where the generalized Porod form $g(q) \sim q^{-(d+n)}$ for the structure factor tail is a consequence of the defect structure, and is independent of the

presence or absence of conservation laws, in systems without defects the functional form does, apparently, differ for conserved and nonconserved systems. We have shown, for example, that for the particular case of the $n=4$ model in two dimensions the tail is well described, over the range of q accessible to us, by a stretched exponential with exponent $\delta=0.435$, differing from the result for the same model with conservation studied by RC [10], who found $\delta\simeq 1.7$.

Within the ''toy'' equation of Bray and Humayun [12], however, we have shown that the true asymptotics are the *same* for conserved and nonconserved dynamics. Of course, the BH equation is at best a large-n theory, and the numerical results for nonconserved and conserved dynamics may converge as n is increased. A related question is whether the exponents δ measured here and in [10] are genuine asymptotic exponents, or effective exponents whose values will change as the range of q over which the fit is made is moved to larger q. More extensive simulations may cast some light on this issue. The ''universal'' (independent of conservation laws) Porod tail behavior obtained for $n\leqslant d$ is geometrical in origin, being a consequence of the field structure induced by singular topological defects [7]. As yet, however, we have no corresponding physical picture in the absence of topological defects.

It is interesting that, within the simple model of equation (4.1), the exponent δ jumps discontinuously from $\delta=2$ at $n=\infty$ to $\delta=1$ for n large but finite. More precisely, one can say that $\delta=2$ corresponds to the limit $n\to\infty$ at fixed, large q, while $\delta=1$ corresponds to $q\to\infty$ at fixed, large n. We have argued that the crossover between these limiting forms for fixed, large n occurs at $q\sim(\ln n)^{1/2}$. This change of behavior depending on the order of the limits is reminiscent of the result obtained from the conserved version of (4.1), where a novel ''multiscaling'' behavior is obtained for $n\to\infty$ at fixed, large t [11], while simple scaling is recovered for $t\to\infty$ at fixed, large n [12]. For the nonconserved case, one always has simple scaling. For both conserved and nonconserved fields, however, the asymptotics of $g(q)$ are sensitive to whether n is large or truly infinite. This rules out, for example, exploring the asymptotics by expanding around the large-n solution in powers of $1/n$.

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APPENDIX

In this Appendix we use (4.6) to derive the asymptotic form (4.7) for $g(q)$. From the definition (4.5) we have

$$B(q)=\frac{1}{n}\int_{\mathbf{p}}\int_{\mathbf{k}} g(\mathbf{p})g(\mathbf{k})g(\mathbf{q}-\mathbf{p}-\mathbf{k}), \tag{A1}$$

where $\int_{\mathbf{p}}\equiv\int d^d p/(2\pi)^d$. Inserting the asymptotic form

$$g(q)\to Aq^{\nu}\exp(-bq^{\delta}), \tag{A2}$$

gives

$$B(q)\to\frac{A^3}{n}\int_{\mathbf{p}}\int_{\mathbf{k}} F(\mathbf{p},\mathbf{k},\mathbf{q})\exp[-bE(\mathbf{p},\mathbf{k},\mathbf{q})], \tag{A3}$$

where

$$F(\mathbf{p},\mathbf{k},\mathbf{q})=|\mathbf{p}|^{\nu}|\mathbf{k}|^{\nu}|\mathbf{q}-\mathbf{p}-\mathbf{k}|^{\nu}$$

$$E(\mathbf{p},\mathbf{k},\mathbf{q})=|\mathbf{p}|^{\delta}+|\mathbf{k}|^{\delta}+|\mathbf{q}-\mathbf{p}-\mathbf{k}|^{\delta}. \tag{A4}$$

We now scale out the q dependence through the changes of variable $\mathbf{p}=q\mathbf{u}$, $\mathbf{k}=q\mathbf{v}$, $\mathbf{q}=q\mathbf{e}$, where $\mathbf{e}$ is a unit vector. Then

$$B(q)=\frac{A^3}{n}q^{2d+3\nu}\int_{\mathbf{u}}\int_{\mathbf{v}} F(\mathbf{u},\mathbf{v},\mathbf{e})\exp[-bqE(\mathbf{u},\mathbf{v},\mathbf{e})]. \tag{A5}$$

For $q\to\infty$, we can attempt to evaluate the $\mathbf{u}$ and $\mathbf{v}$ integrals using the method of steepest descents. This requires minimizing the function $E(\mathbf{u},\mathbf{v},\mathbf{e})$. The points requiring consideration are the symmetry point, $\mathbf{u}=\mathbf{v}=\mathbf{e}/3$, and the points $\mathbf{u}=\mathbf{0}=\mathbf{v}$ and two similar points obtained by permuting $\mathbf{u}$, $\mathbf{v}$, and $\mathbf{e}-\mathbf{u}-\mathbf{v}$. The corresponding values of E are $E(\mathbf{e}/3,\mathbf{e}/3,\mathbf{e}/3)=3^{1-\delta}$, and $E(\mathbf{0},\mathbf{0},\mathbf{e})=E(\mathbf{0},\mathbf{e},\mathbf{0})=E(\mathbf{e},\mathbf{0},\mathbf{0})=1$. Thus for $\delta>1$, the symmetry point minimizes E, giving $B(q)\sim\exp(-3^{1-\delta}bq)$. But this form violates the asymptotic relation (4.6), according to which $B(q)$ and $g(q)$ must decay with the *same* exponential factor, so $\delta>1$ is ruled out.

For $\delta<1$, the smallest E is unity, obtained when two of $\mathbf{u}$, $\mathbf{v}$, and $\mathbf{e}-\mathbf{u}-\mathbf{v}$ vanish. So this case is apparently consistent with (4.6). However, the integral is now dominated by points where two of the momenta $\mathbf{p}$, $\mathbf{k}$, and $\mathbf{q}-\mathbf{p}-\mathbf{k}$ vanish. This invalidates the use of the asymptotic form for $g(q)$ in the evaluation of $B(q)$, so the derivation of a stretched exponential form is not internally consistent for $\delta<1$.

This leaves $\delta=1$. For this case all points of the form $\mathbf{u}=\alpha\mathbf{e}$, $\mathbf{v}=\beta\mathbf{e}$, with $0\leqslant\alpha\leqslant 1$ and $0\leqslant\beta\leqslant 1-\alpha$, give $E=1$, so one has to integrate over all such points. Writing $\mathbf{u}=\alpha\mathbf{e}+\mathbf{u}_{\perp}$, $\mathbf{v}=\beta\mathbf{e}+\mathbf{v}_{\perp}$, expanding E to quadratic order in $\mathbf{u}_{\perp}$, $\mathbf{v}_{\perp}$, and carrying out the integrals over $\mathbf{u}_{\perp}$, $\mathbf{v}_{\perp}$, gives after some algebra

$$B(q)=(A^3/4\pi^2 n)q^{d+1+3\nu}\exp(-bq)I(d,\nu)/(2\pi b)^{d-1}$$

$$I(d,\nu)=\int_0^1 d\alpha\int_0^{1-\alpha} d\beta[\alpha\beta(1-\alpha-\beta)]^{\nu+(d-1)/2}. \tag{A6}$$

But (4.6) implies, asymptotically,

$$B(q)=(2A/\lambda)q^{2+\nu}\exp(-bq). \tag{A7}$$

Comparing (A6) and (A7) gives $\nu=(1-d)/2$ and Eq. (4.8) for the amplitude A.

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