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Phase-ordering dynamics of systems with a conserved vector order parameter

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We study the dynamic scaling properties of systems with a conserved order parameter with O(n) symmetry, using the Gaussian auxiliary field approach of Mazenko [Phys. Rev. Lett. **63**, 1605 (1989); Phys. Rev. B **42**, 4487 (1990); **43**, 5747 (1990)]. Results valid in the limit of large n, and for finite n, are presented. An explicit numerical solution to the full fourth-order nonlinear equation for the real-space scaling function $f(x)$ is obtained by truncating the equation at leading nontrivial order in $1/n$. In Fourier space the results are in very good agreement, for n as small as 5, with approximate analytic results for the scaling structure deduced by Bray and Humayun [Phys. Rev. Lett. **68**, 1559 (1992)] from a large-n analysis. Two approximate schemes have been introduced to treat the finite-n problem. The first, an expansion to order f^3, reduces the differential equation to one that is similar to the $1/n$ expansion, with n replaced by an effective n^*. The scaling function and structure factor for $n = 2$, $d = 3$ are in excellent agreement with recent simulation results. This approach respects the conservation law, but the correct large-q behavior ("Porod's law") of the structure factor is not recovered. In the second scheme, the large-q tail is recovered at the cost of violating (weakly) the conservation law. The real-space scaling function has the same qualitative features as the simulation results for $n = 2$, $d = 3$, but is not as quantitatively accurate as the previous approach. For $n \geq 5$, both schemes produce very similar results.

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I. INTRODUCTION

The dynamics of phase separation in systems quenched from a high temperature disordered state into an ordered region of the phase diagram is an area of great activity [1].

Recently, there has been an increasing interest in the study of the dynamics of phase ordering in systems with more complicated symmetries, e.g., the O(n) model, which is described by an n-component vector order parameter [2, 3]. One approach that has been successfully applied in recent years to study such systems is the Gaussian auxiliary field method introduced by Mazenko [4], following earlier work by Ohta, Jasnow, and Kawasaki for nonconserved scalar fields [5]. This approach allows one to find an approximate closed equation for the evolution of the pair correlation function for the order parameter field. Although the dynamic scaling properties of systems with nonconserved order parameter have recently been studied [2] using this approach, much less is known for the corresponding properties in systems with conserved order parameter. The aim of the present paper is to use the Gaussian field method to explore the dynamical scaling properties of systems described by a conserved vector order parameter.

A central concept in the dynamics of phase ordering is the characteristic length scale $L(t)$, which grows with time as a power of the form $L(t) = t^{1/z}$. The value of the dynamical exponent z has been determined by Bray using a renormalization group (RG) analysis [6], with the result $z = 3$ for a conserved scalar order parameter, confirming earlier predictions, whereas $z = 4$ for a conserved vector order parameter. Recent work by Bray and Rutenberg (BR), using an "energy scaling" argument [7], recovers all the RG results but with an extra logarithm for conserved fields with $n = 2$, which is a marginal case in the RG analysis. Thus BR predict $L(t) \sim (t \ln t)^{1/4}$ for $n = 2$ (and $d > 2$), while $L(t) \sim t^{1/4}$ for $n > 2$.

A consequence of the assumption that $L(t)$ is the only characteristic scale at late times (the "dynamic scaling hypothesis") is that the two-point correlation function of the order parameter, $C(\mathbf{r}, t) = \langle \phi(\mathbf{x}, t)\phi(\mathbf{x}+\mathbf{r}, t)\rangle$, where $\langle\,\rangle$ indicates an average over both initial conditions and thermal noise, takes the scaling form

$$C(\mathbf{r}, t) = f(r/L(t)) , \tag{1}$$

while its Fourier transform, the structure factor, which can be measured in scattering experiments, has the corresponding scaling form

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

where $g(y)$ is the Fourier transform of $f(x)$. One remaining issue is to determine the shapes of the scaling functions and their properties for systems with continuous symmetry, when the order parameter is a conserved vector quantity.

Coniglio and Zannetti (CZ) [8] solved the conserved O(n) model exactly in the large-n limit. They found that the structure factor does not exhibit the standard dynamic scaling form (2). Instead, they find a "multiscaling" solution with two, logarithmically different, diverging length scales. It should be noted that the CZ solution is strictly valid for $n = \infty$. Bray and Humayun (BH) [9], using the Gaussian auxiliary field method of Mazenko, showed that introducing the $1/n$ correction to the equation of motion removes the multiscaling and the standard scaling solution is recovered. They also derived an expression for the scaling structure factor valid for large, but finite, n.

In recent work, Siegert and Rao (SR) [10] simulated numerically a Langevin equation for a three-dimensional XY model ($n = 2$) with conserved order parameter. Their results show no indication of multiscaling, being consistent with standard scaling and the known value, $z = 4$, of the dynamic exponent. Indeed, a reanalysis of their data [11] shows excellent agreement with the $(t \ln t)^{1/4}$ growth predicted by BR. Moreover, they note that the real-space scaling function is already quite well described by the large-n form of BH.

In the first part of the present work, we extend the analysis of BH, solving the full nonlinear differential equation for the scaling function $f(x)$, truncated at order $1/n$, but without the restriction that n must be large. Our results are compared with the analytical solutions for the structure factor deduced by BH. The results are well described by an approximate form [Eq. (21)] for the scaling function $g(q)$, motivated by the large-n result of BH.

In the second part, using the equation for the correlation function, which depends on the second moments of the Gaussian field, we derive a closed equation for the correlation function C for finite n up to order C^3. The $O(C^3)$ term is the leading correction that must be included in order to recover standard scaling. In particular, for the case $n = 2$ our results are in excellent agreement with the simulation results of SR. Finally, the finite-n case is reconsidered in order to introduce the correct asymptotic behavior ("Porod's law" [2, 12–14]) in the structure factor. This is done by solving the differential equation for the correlation function of the Gaussian auxiliary field, and using the result in the mapping function that relates it to correlation function for the physical field. This mapping function feeds in the information related to topological defects in the system, these defects being responsible for the Porod tail in the structure factor.

II. MAZENKO'S APPROACH

A closed equation for the order-parameter correlation function can be obtained using the Gaussian auxiliary field method introduced by Mazenko [4]. The application of this approach to conserved vector fields is a straightforward extension of the nonconserved case [2]. We begin with the equation of motion for conserved order parameter with continuous symmetry,

$$\frac{\partial \boldsymbol{\phi}(1)}{\partial t_1} = -\nabla^2 \left(\nabla^2 \boldsymbol{\phi}(1) - \frac{\partial V(\boldsymbol{\phi}(1))}{\partial \boldsymbol{\phi}(1)} \right) , \qquad (3)$$

where 1 represents the space-time point (x_1, t_1), and $V(\boldsymbol{\phi})$ is a generalized potential with ground state given by a manifold connected by rotations. The $n = 2$ case is the well-known "Mexican hat" potential. Taking the scalar product of Eq. (3) with $\boldsymbol{\phi}(2)$ [the order parameter at the point (x_2, t_2)] and taking the average over the ensemble of initial conditions yields

$$\frac{\partial C(12)}{\partial t_1} = -\nabla_1^2 \left(\nabla_1^2 C(12) - \left\langle \frac{\partial V(\boldsymbol{\phi}(1))}{\partial \boldsymbol{\phi}} \cdot \boldsymbol{\phi}(2) \right\rangle \right) . \qquad (4)$$

Translational invariance ensures that the two-point, two-time correlation function $C(12) = \langle \boldsymbol{\phi}(1) \cdot \boldsymbol{\phi}(2) \rangle$ depends on the spatial coordinates only through $r = |x(1) - x(2)|$.

The key idea in the Mazenko approach is to introduce a Gaussian auxiliary field $\mathbf{m}$, which is related to $\boldsymbol{\phi}$. Then it is possible to calculate the average on the right-hand side of Eq. (4). In the late stages of growth, the order parameter $\boldsymbol{\phi}$ will lie on the ground state manifold except in the neighborhood of topological defects. A convenient choice for the auxiliary field is defined by the solution of the differential equation $\nabla_m^2 \boldsymbol{\phi} = \partial V(\boldsymbol{\phi})/\partial \boldsymbol{\phi}$, with the boundary conditions $\boldsymbol{\phi}(0) = 0$ and $\boldsymbol{\phi} = \hat{\mathbf{m}} = \mathbf{m}/|\mathbf{m}|$ as $\mathbf{m} \to \infty$. Then the vector $\mathbf{m}$ can be regarded as a coordinate in space normal to the defect. With the assumption that $\mathbf{m}$ can be approximated by a Gaussian random field, the average in the second term of the right-hand side of Eq. (4) can be evaluated to give [2]

$$\frac{\partial C}{\partial t} = -\nabla^2 \left(\nabla^2 C + \alpha(t) \gamma \frac{dC}{d\gamma} \right) , \qquad (5)$$

where $\alpha(t) = \langle m(1)^2 \rangle^{-1}$, the inverse of the second moment of one component of $\mathbf{m}$, and

$$\gamma \equiv \gamma(12) = \langle m(1) m(2) \rangle / \{ \langle [m(1)]^2 \rangle \langle [m(2)]^2 \rangle \}^{1/2}$$

is the normalized two-point correlation function of m.

The relation between C and γ is obtained from $C(12) = \langle \hat{\mathbf{m}}(1) \cdot \hat{\mathbf{m}}(2) \rangle$. The detailed calculation was done in [2, 12, 13] and the final result is

$$C = \frac{n\gamma}{2\pi} \left[B \left(\frac{n+1}{2}, \frac{1}{2} \right) \right]^2 F \left(\frac{1}{2}, \frac{1}{2}; \frac{n+2}{2}, \gamma^2 \right) , \qquad (6)$$

where $B(x, y)$ is the beta function and $F(a, b, c; z)$ is the hypergeometric function.

Equations (5) and (6) define a closed set of equations for the correlation function. The simplest way to proceed is to rewrite Eq. (5) as an equation for γ and solve it numerically. The solution is put back into (6) to finally obtain the correlation function. One important feature is that a scaling solution to Eq. (5) captures the correct characteristic length $L(t) = t^{1/4}$, and requires $\alpha(t) \sim t^{-1/2}$. [However, it fails to pick up the expected logarithm in $L(t)$ [7] for $n = 2$, while the derivation of the $t^{1/3}$ growth for scalar fields using this approach requires an explicit introduction of the bulk diffusion field [4].]

III. $1/n$ EXPANSION

In the large-n limit further progress can be made, from Eq. (6), by performing an expansion in $1/n$. This gives $C = \gamma - \gamma(1-\gamma^2)/2n + O(1/n^2)$, implying $\gamma dC/d\gamma = C + C^3/n + O(1/n^2)$. Thus (5) becomes a closed equation for C. For the *equal-time* correlation function, an additional factor of $1/2$ is required in front of the time derivative, giving, correct to $O(1/n)$,

$$\frac{1}{2}\frac{\partial C}{\partial t} = -\nabla^2 \left[\nabla^2 C + \alpha(t)\left(C + \frac{C^3}{n}\right)\right]. \qquad (7)$$

The alert reader may notice the original motivation behind this approach, namely, the inclusion in a natural way of the appropriate topological defects, seems to be lost for large n, since there are no stable singular defects for $n > d$. Nevertheless, Eq. (7) seems to capture much of the important physics. In particular, the nonlinearity inherent in (5) for finite n is essential in recovering conventional scaling. In Sec. IV we will show that expanding in C, with n arbitrary, gives an equation of the same form as (7) but with n replaced by an effective value n^*. Furthermore, including only the leading nonlinearity gives very good agreement with the simulation results of SR for $d = 3$, $n = 2$. First, however, we consider the case of n strictly infinite.

A. Multiscaling solution for $n = \infty$

The limit $n \to \infty$ in Eq. (7) leads to the equation solved by CZ and its solution gives rise to multiscaling behavior. The CZ equation can easily be solved in Fourier space for the structure factor $S(\mathbf{k}, t)$. This is given by

$$\frac{1}{2}\frac{dS(\mathbf{k},t)}{dt} = -[k^4 - k^2\alpha(t)]S(\mathbf{x},t). \qquad (8)$$

The solution is $S(\mathbf{k},t) = \Delta \exp[r(k,t)]$, where $r(k,t) = -2k^4 t + 2k^2\beta(t)$ with $\beta(t) = \int_0^t dt'\,\alpha(t')$ determined self-consistently from the condition $\sum_k S(\mathbf{k},t) = 1$. The initial condition Δ is assumed to be independent of k.

For large t, the sum is dominated by values of k close to k_m, the maximum of $r(k,t)$, where the structure factor is sharply peaked. It can be evaluated using the method of steepest descent, giving $k_m = [\beta(t)/2t]^{1/2}$ and $r(k_m,t) = \beta^2(t)/2t$. Expanding the summand around k_m, using $r(k,t) = \beta^2(t)/2t - 4\beta(k-k_m)^2 + \cdots$, and integrating, we find that the condition for $\beta(t)$ is

$$1 = C_0 \left(\frac{\beta^2}{2t}\right)^{\frac{d-2}{4}} t^{-\frac{d}{4}} \exp\left(\frac{\beta^2}{2t}\right), \qquad (9)$$

where C_0 is a constant whose explicit value is not relevant, and d is the spatial dimension. Solving the above equation for large t, the region of interest, gives

$$\beta(t) \simeq \left(\frac{dt}{2}\ln t\right)^{\frac{1}{2}}, \qquad (10)$$

implying

$$k_m \simeq \left(\frac{d}{8}\frac{\ln t}{t}\right)^{\frac{1}{4}}. \qquad (11)$$

Finally, the structure factor can be written, up to constants, as

$$S(k,t) \simeq (\ln t)^{\frac{2-d}{4}}\, L(t)^{d\phi(\frac{k}{k_m})}, \qquad (12)$$

with $\phi(x) = 1 - (x^2-1)^2$. Thus $S(k,t)$ depends on two, logarithmically different, length scales: $L(t) = t^{1/4}$ and $k_m^{-1} \simeq (8t/d\ln t)^{1/4}$. Equation (12) represents "multiscaling" behavior [8] because the exponent of $L(t)$ depends continuously on the ratio k/k_m.

B. Scaling solution for finite n

Here we show that retaining the $O(1/n)$ term in (7) leads to a solution in the standard scaling form. We summarize briefly the analysis of BH, as it provides the framework for the rest of the paper. If (7) is written in terms of the scaling function $f(x)$ defined by Eq. (1), with $L(t) = t^{1/4}$, and the Fourier transform is taken, the following equation for the scaling function $g(q)$ [the Fourier transform of $f(x)$] defined by Eq. (2) is obtained:

$$\frac{dg}{dq} = -\left(\frac{d}{q} + 8q^3 - 8q_m^2 q\right) g + qB(q). \qquad (13)$$

Here $B(q) = 8q_m^2(f^3)_q/n$, $(f^3)_q$ means the (d-dimensional) Fourier transform of $f^3(x)$, and $\alpha(t)$ in (7) was written as $q_m^2/t^{1/2}$ consistent with $t^{1/4}$ growth. We will see that q_m is the position of the maximum in $g(q)$.

BH showed that for $n = \infty$, when the $B(q)$ term is dropped, the attempt to find a scaling solution fails due to a nonintegrable q^{-d} singularity in $g(q)$ at small q. The absence of a scaling solution in this limit agrees with the CZ result. But for any finite n, no matter how large, a standard scaling solution is consistent with (13). A formal integration of (13), with initial condition $g(0) = 0$ (as required by the conserved dynamics), gives

$$g(q) = q^{-d}\exp(-2q^4 + 4q_m^2 q^2) \times \int_0^q dq'\, q'^{d+1} B(q') \exp(2q'^4 - 4q_m^2 q'^2). \qquad (14)$$

For $q \to 0$ the integral is sensible, giving $g(q) \simeq B(0)q^2/(d+2)$ where $B(0) = (8q_m^2/n)\int d^dx\, f^3(x)$, which is nonzero.

BH show that $q_m \to \infty$ for $n \to \infty$, and use this property to evaluate the integral. For large q_m the integral will be dominated by q' of order $1/q_m$, provided $1/q_m \ll q < \sqrt{2}q_m$ [which includes the vicinity of the maximum in $g(q)$, at $q = q_m$]. Then the $q_m^2 q'^2$ term in the exponential factor in the integrand dominates the q'^4 term, so we can replace $B(q')$ by $B(0)$ and extend the upper limit of the integral to infinity. This gives

$$g(q) = 2^{-(d+3)}\,\Gamma\left(1 + \frac{d}{2}\right) B(0) q_m^{-(d+2)} q^{-d} \times \exp(-2q^4 + 4q_m^2 q^2), \qquad (15)$$

which is valid in the interval $1/q_m \ll q < \sqrt{2}q_m$. In essence this is a large-n solution.

The constant q_m is determined by the condition that $f(0) = 1$ or equivalently $\sum_q g(q) = 1$. The sum is evaluated by steepest descent and the condition is

$$1 = 2^{-(d+5)}\sqrt{2\pi}k_d\Gamma\left(1 + \frac{d}{2}\right) q_m^{-(d+4)} \exp(2q_m^4) B(0), \qquad (16)$$

where $k_d = 2/[\Gamma(d/2)(4\pi)^{d/2}]$. This equation relates q_m and $B(0)$. Substituting $B(0)$ from Eq. (16) into Eq. (15), the final form for the structure factor is obtained:

$$g(q) = \frac{4}{k_d\sqrt{2\pi}}\, q_m^2 q^{-d} \exp[-2(q^2 - q_m^2)^2]. \tag{17}$$

We stress that this is valid for $1/q_m \ll q < \sqrt{2}q_m$.

When $q_m \to \infty$ the function (17) becomes a properly normalized δ function:

$$g(q) \to k_d^{-1} q_m^{1-d} \delta(q - q_m)\ , \tag{18}$$

and the real-space scaling function takes the form

$$f(x) = 2^\nu \Gamma(\nu + 1) \frac{J_\nu(q_m x)}{(q_m x)^\nu}, \tag{19}$$

with $\nu = (d-2)/2$ and J_ν the Bessel function.

Finally $B(0) = 8q_m^2 \int d^dx f(x)^3/n \approx c_d\, q_m^{2-d}/n$, with c_d a constant. Using this result in (16) gives a closed equation for q_m, valid for large q_m, with solution $q_m \sim [(\ln n)/2]^{1/4}$.

We have noted that (17) is a representation of a spherical δ function, as in (18), for $q_m \to \infty$. Another representation is the Gaussian form to which (17) reduces for $|q - q_m| \ll q_m$, i.e.,

$$g(q) = \frac{4}{k_d\sqrt{2\pi}} q_m^{2-d} \exp[-8q_m^2\, (q - q_m)^2]\ . \tag{20}$$

Since $g(q)$ is vanishingly small when $|q - q_m| \gg 1/q_m$, this form should be accurate for large q_m. Note, however, that since q_m grows very slowly with n, i.e., $q_m \sim [(\ln n)/2]^{1/4}$, extraordinarily large-$n$ values are required to achieve quite moderate values of q_m, e.g., $q_m = 10$ requires $n \sim 10^{8686}$. In practice, therefore, the difference between (17) and (20) will be important when fitting data for all reasonable values of n. The most obvious difference is an asymmetry about $q = q_m$ in (17): the function decreases more rapidly for $q > q_m$ than for $q < q_m$.

These two functions play a large role in our following discussions. First, let us consider the more general forms

$$g_1(q) = A \exp\left(-\frac{(q^2 - q_m^2)^2}{2\sigma^2}\right) \tag{21}$$

and

$$g_2(q) = A \exp\left(-\frac{(q - q_m)^2}{2\sigma^2}\right)\ . \tag{22}$$

We have introduced three adjustable parameters, the amplitude A, the position q_m of the maximum, and some measure σ of the width. Since the real-space scaling function satisfies $f(0) = 1$, only two of these are independent. The particular choice (22) has the advantage that its Fourier transform can be evaluated analytically for $q_m \gg \sigma$,

$$f(x) = f_0 \exp\left(-\frac{1}{2}\frac{\rho^2}{\lambda^2}\right) \sqrt{1 + \left(\frac{\rho}{\lambda^2}\right)^2}\, \frac{\sin(\rho + \phi)}{\rho}, \tag{23}$$

where $\rho = q_m x$, $\lambda = q_m/\sigma$, $f_0 = [1 + 1/\lambda^2]^{-1}$, and $\phi = \tan^{-1}(\rho/\lambda^2)$. This form is valid for $\lambda \gg 1$: the error is of order $\exp(-\lambda^2/2)$. By contrast, Eq. (21) does not have a simple analytic form in real space. We shall find, however, that it gives a significantly better fit to structure-factor data than (22).

In the limit of large n, comparison of (21) and (22) with (17) and (20), respectively, suggests that $1/2\sigma^2$ should approach 2 and $8q_m^2$, respectively.

C. Real-space scaling analysis

For a real-space analysis, we return to Eq. (7). Setting $\alpha(t) = \alpha/t^{1/2}$, and $C(\mathbf{r}, t) = f(r/t^{1/4})$, (7) becomes

$$\frac{1}{8} x \frac{df}{dx} = \nabla_x^2 \left[\nabla_x^2 f + \alpha\left(f + \frac{f^3}{n}\right)\right], \tag{24}$$

where $\nabla_x^2 = \left(\frac{d^2}{dx^2} + \frac{d-1}{x}\frac{d}{dx}\right)$.

In principle, we would like to solve the full nonlinear equation (5), with $C(\gamma)$ given by (6). In practice, however, the solution presents formidable numerical difficulties [mainly associated with the singularity of $C(\gamma)$ at $\gamma = 1$], which we have not been able to overcome satisfactorily. Instead, therefore, we address initially the simpler problem of solving (24), in which the right-hand side of (5) has been expanded to order $1/n$, the lowest order consistent with simple scaling. However, we will no longer regard n as large in (24), but solve numerically for general values of n. In practice, a minor modification of this procedure (see Sec. IV), in which n is replaced by an effective value n^*, gives results in good agreement with simulations even for $n = 2$.

The fourth-order nonlinear equation (24) must be solved with the appropriate boundary conditions. Small- and large-x analyses enable one to obtain the boundary conditions at $x = 0$ and the asymptotic behavior. Inserting a power series solution of the form $f(x) = 1 + \sum_{r=1} \beta_r\, x^r$, and keeping terms to order x^4, we obtain the expansion $f(x) = 1 + \beta\, x^2 - (1 + 3/n)\alpha\beta\, x^4/4(d+2) + \cdots$ where β_2 has been redefined as β. So, the required four boundary conditions for the numerical integration of the fourth-order equation are $f(0) = 1$, $f'(0) = 0$, $f''(0) = 2\beta$, $f'''(0) = 0$, where the parameter β is, however, undetermined.

Since $f(x)$ vanishes for large x, the large-x solution can be obtained from the linearized version of (24). Of the four linearly independent solutions, one is $f(x) = \text{const}$, while the other three include two physical solutions, whose asymptotic forms (correct to the leading exponential terms) can be combined as

$$f(x) \approx A \exp(-3x^{4/3}/16) \cos(3\sqrt{3}x^{4/3}/16 + \phi)$$

(with ϕ an arbitrary phase), and one unphysical exponentially growing solution, $f(x) \approx B \exp(3x^{4/3}/8)$.

Our equation has two undetermined parameters, α and β, the latter entering through the boundary conditions. As the scaling function $f(x)$ must vanish at $x = \infty$, these two parameters are determined by the boundary condition that the unphysical constant and exponentially growing solutions of the linearized equation should be absent at large x. Thus the problem is defined as a nonlinear eigenvalue equation, with eigenvalues α and β. A similar situation is familiar from the analogous treatment of nonconserved fields [2], but with only one eigenvalue to determine in that case. The two-eigenvalue case is also encountered for conserved scalar fields [4].

The existence of an increasing exponential makes the eigenvalue determination more difficult, and the standard numerical procedures are not suitable for this problem. We therefore follow the heuristic numerical procedure described by Mazenko [4], when he treats the conserved scalar case. Applying this method it is possible to find the pair of eigenvalues for any n and determine the scaling function shape.

In this part of the work we solve Eq. (24) for several values of n to determine the relevant features of the scaling function $f(x)$. In addition, we make a close comparison of the structure-factor scaling function $g(q)$ with expressions (21) and (22), motivated by the work of BH.

D. Results and discussion

We have solved Eq. (24) for $n = 5$, 20, and 50 in three dimensions. Consider first the case $n = 5$. In Table I we give the eigenvalues α and β, together with results for the zeros and turning points of $f(x)$. Figure 1(a) is a plot of $f(x)$. An analysis in Fourier space allows a comparison with the BH results. Figure 1(b) shows the corresponding structure-factor scaling function $g(q)$ (continuous line) obtained by numerical Fourier transformation of $f(x)$. As the width is finite, the δ-function approximation is not adequate in this case. Instead, we use the quartic exponential and Gaussian forms Eqs. (21) and (22). We fit these functions to the numerical structure factor using a nonlinear least-squares algorithm. The full set of best-fit parameters for the three n values considered is presented in Table IV. The relation between the three adjustable parameters, imposed by the real-space condition $f(0) = 1$, is satisfied to within 3% for $n = 5$, and to within 1% for $n = 20$ and 50.

TABLE I. Information on the scaling function, for $n = 5$, extracted numerically in the $1/n$ approximation. The eigenvalues are $\alpha = 1.727\,434\,47$ and $\beta = -0.317\,977\,5$.

Quantity	x	$f(x)$
First zero	2.512	0
First minimum	3.501	-0.146124
Second zero	5.025	0
Second maximum	5.998	0.049786
Third zero	7.433	0
Second minimum	8.372	-0.017997

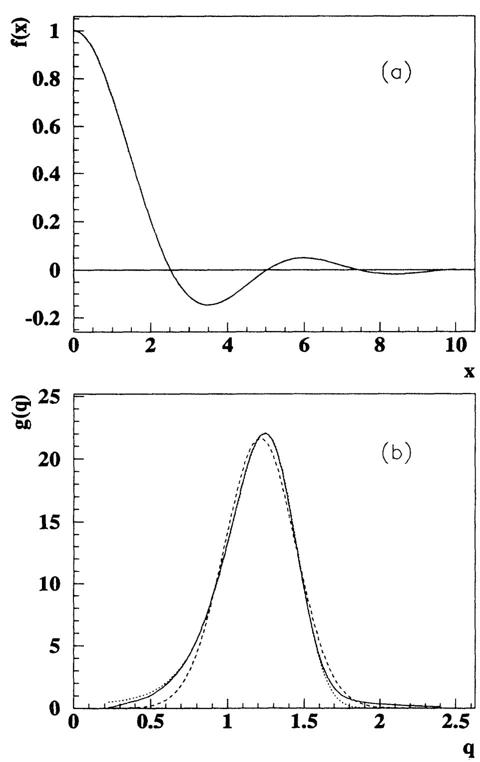

FIG. 1. (a) Scaling function for $n = 5$ in the $1/n$ approximation of Sec. III C. (b) The structure factor (continuous line) and the best fits to the Gaussian (long dash line) and the quartic exponential (small dash line) forms (22) and (21).

Continuing with the $n = 5$ discussion, Fig. 1(b) shows the best fits to the Gaussian (long dash line) and quartic exponential (short dash line). The latter, motivated by the BH large-n analysis, clearly gives a much better fit.

One particular feature that has not been considered in the analytical treatment is the asymptotic behavior of the structure factor for finite n. As can be observed in Fig. 1(b), the large-q tail of the structure factor seems to be decaying more slowly than either the Gaussian or quartic exponential fits. The origin of this feature is not clear. Note that it is not related to the Porod tail [2, 12–14], $g(q) \sim 1/q^{d+n}$, present in the solution of the full equation (5), since the approximate equation (24) does not possess the short-distance singularity responsible for the tail. An approximate treatment that does incorporate the Porod tail will be given in Sec. V.

For $n = 20$ and 50, the relevant numerical features of the scaling function are detailed in Tables II and III. The scaling functions for $n = 20$ and 50 are presented in Figs. 2(a) and 3(a), respectively, while Figs. 2(b) and 3(b) give the corresponding structure factors together with the best fits to Eqs. (21) and (22). For these larger values

TABLE II. Information on the scaling function, for $n = 20$, extracted numerically in the $1/n$ approximation. The eigenvalues are α=2.017 482 70 and $\beta = -0.329\,225\,0$.

Quantity	x	$f(x)$
First zero	2.349	0
First minimum	3.2739	-0.169990
Second zero	4.656	0
Second maximum	5.597	0.067340
Third zero	6.913	0
Second minimum	7.832	-0.028345

TABLE III. Information on the scaling function, for $n = 50$, extracted numerically in the $1/n$ approximation. The eigenvalues are α=2.179 330 049 and $\beta = -0.348\,712\,5$.

Quantity	x	$f(x)$
First zero	2.243	0
First minimum	3.147	-0.179053
Second zero	4.463	0
Second maximum	5.383	0.075650
Third zero	6.641	0
Second minimum	7.545	-0.034130

of n, the fits to the quartic exponential form (21) are exceptionally good, and almost indistinguishable from the continuous curves obtained from the numerical solution of (24).

What the above solutions show is that the quartic exponential gives a very good fit to the numerical results—much better than a simple Gaussian. It should be noted that, with either of these functions, there is weak violation of the conservation law, because they do not vanish at $q = 0$. The violation is worse for the quartic exponential, which has the value $g_1(0) = A\exp(-{q_m}^4/2\sigma^2)$. For $n = 5$ the absolute error is $g_1(0) = 0.385$, while the corresponding results for $n = 20$ and 50 are 0.065 and 0.017, respectively. On the other hand, dividing the absolute error by the peak value A of the structure factor gives relative errors of 0.017, 3×10^{-3}, and 8×10^{-4} for $n = 5$, 20, and 50, respectively. For the Gaussian fit, the violation of the conservation law is much weaker, but quality of the overall fit is considerably poorer.

At the end of Sec. III B we noted that comparison with the analytic large-n result of BH suggests that the quantity $1/2\sigma^2$ in the fitting functions $g_1(q)$ and $g_2(q)$, defined by Eqs. (21) and (22), should approach the values 2 and $1/8q_m^2$, respectively, for large n. From the right side of Table IV we see that for the quartic exponential fit, $1/2\sigma^2$ does indeed seem to be approaching 2, although the convergence is rather slow. From the left side of the table we find, for the Gaussian fit, that $8q_m^2$ takes the values 11.78, 14.02, and 15.50 for $n = 5$, 20, and 50, respectively, again getting closer to $1/2\sigma^2$ for larger n. The slow convergence is associated with the slow growth (with n) of q_m, which increases only as $(\ln n)^{1/4}$ for $n \to \infty$.

IV. C^3 EXPANSION FOR FINITE n: THE CASE $n = 2$

As an alternative to the expansion to order $1/n$, we consider in this section a direct expansion of the full non-

TABLE IV. Parameters determined from the Gaussian and quartic exponential fits, in the $1/n$ approximation for several values of n.

	Gaussian			Quartic exponential		
n	A	$1/2\sigma^2$	q_m	A	$1/2\sigma^2$	q_m
5	21.6374	9.3172	1.2133	22.0187	1.6830	1.2452
20	21.4899	11.9650	1.3237	21.6862	1.7463	1.3503
50	21.0019	13.5572	1.3920	21.1538	1.7848	1.4115

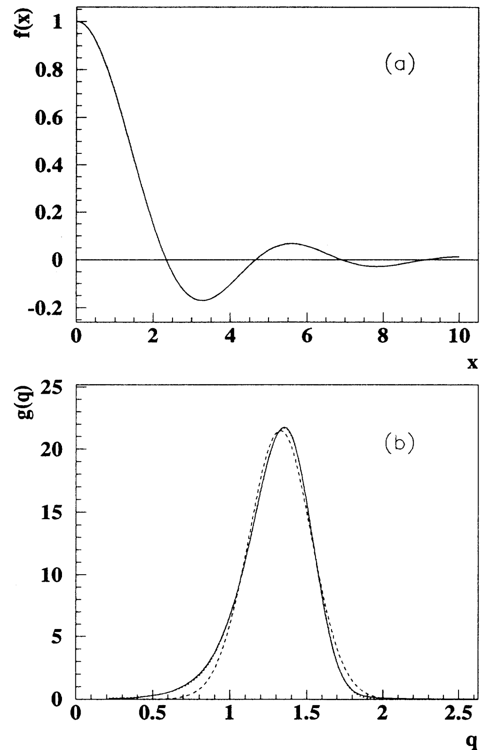

FIG. 2. (a) Same as Fig. 1(a), but for $n = 20$. (b) Same as Fig. 1(b), but for $n = 20$.

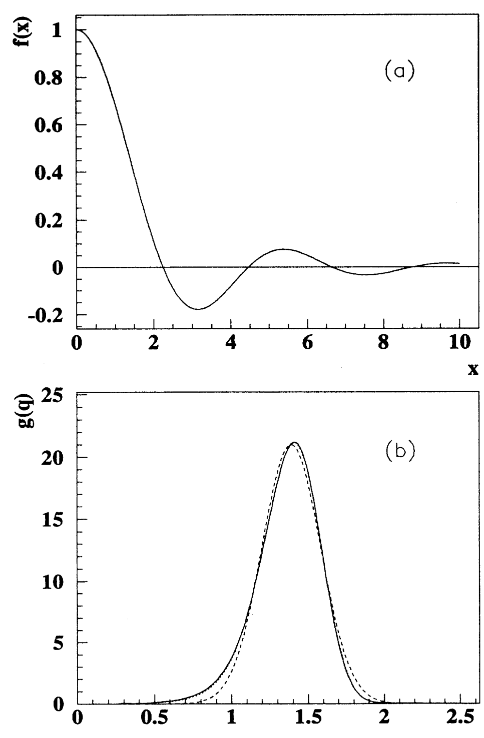

FIG. 3. (a) Same as Fig. 1(a), but for $n = 50$. (b) Same as Fig. 1(b), but for $n = 50$.

linear equation (5) to leading nontrivial order in the correlation function C, i.e., to order C^3. (We recall that an expansion beyond linear order is necessary to recover standard scaling.) The motivation behind this approach is that one might hope to use it for quite small values of n, in particular the case $n = 2$ which was studied numerically by SR [10]. In practice, of course, the resulting equation for $f(x)$ has a form identical to (24), except that the coefficient of the f^3 term is no longer simply $1/n$.

SR argued that their solution for the scaling function is well modulated by the large-n form $f(x) = \sin(q_m x)/q_m x$ found by BH. This is our main motivation for studying the finite-n case in this approximation. If we introduce the leading nonlinear term in the equation for C for fixed, finite n the equation will be identical in structure to that studied in Sec. III. To obtain the expansion, we proceed as follows. First, expand Eq. (6) for C to order γ^3: $C(\gamma) = a_n\gamma\,[1 + \gamma^2/2(n+2) + O(\gamma^4)]$, with $a_n = n[B((n+1)/2, 1/2)]^2/2\pi$. Next, we evaluate the final term in (5), $\gamma\, dC/d\gamma = a_n\gamma[1+3\gamma^2/2(n+2)+O(\gamma^4)]$. Finally we eliminate γ between C and $\gamma\, dC/d\gamma$ to obtain $\gamma\, dC/d\gamma = C + C^3/n^* + O(C^5)$, with $n^* = (n+2)\, a_n^2$.

This equation is the same as that studied in the preceding section, but here there is an effective n^*. Of course, in the limit $n \to \infty$, $n^* \to n$, and we recover the limit studied before. Numerical solution in the real-space scaling variable is the most convenient way of proceeding.

In order to compare our results with the simulations of SR, we will consider specifically the case $n = 2$, $d = 3$. For $n = 2$, the effective n is $n^* = \pi^2/4 = 2.4674\ldots$. Solving the equation as described before, one can find the scaling solution. Table V gives the positions of the zeros and turning points. In Fig. 4(a) a plot of the scaling function is presented, with the abscissa rescaled so that the first zero of $f(x)$ is at $x = 1$. The simulation data of SR, scaled in the same way, are included in the figure. Considering the relative crudeness of the C^3 approximation, the agreement is remarkably good. In particular, the positions of the higher-order zeros, and the positions and amplitudes of the turning points, are well represented.

Another interesting feature of the numerical solution is the existence of a quite slowly decaying large-q tail in the structure factor, which fits the data reasonably well. In fact it can be shown that the full theory, represented by Eq. (5), generates the correct "Porod tail," of the form $g(q) \sim q^{-(d+n)}$. This is related to a corresponding singular term of the form $|x|^n$ (with an additional logarithm for n even) in the short-distance expansion for $f(x)$ [2, 12]. In order to generate this singular term, however, it is necessary to retain the full nonlinear term $\gamma dC/d\gamma$ in (5), the singularity at small x being associated with the singularity of the hypergeometric function (6) at $\gamma = 1$. This singularity is lost when the hypergeometric function is truncated at $O(C^3)$, and with it the Porod tail. The appearance of a slowly decaying tail in the numerical solution is, therefore, slightly mysterious. We have been unable to determine analytically the asymptotic form for the truncated equation.

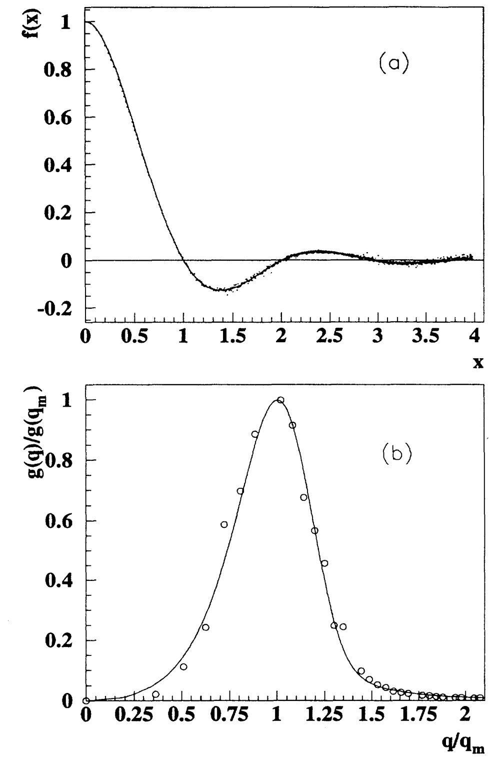

FIG. 4. (a) Scaling function for $n = 2$ in the C^3 approximation of Sec. IV. The data points are the simulation data of Siegert and Rao [10]. (b) The corresponding structure factor. The data points are from Ref. [10].

TABLE V. Information on the scaling function, for $n = 2$ ($n^* = \pi^2/4$), extracted numerically in the C^3 approximation. The eigenvalues are $\alpha = 1.548\,804\,350$ and $\beta = -0.333\,625\,0$.

Quantity	x	$f(x)$
First zero	2.619	0
First minimum	3.623	-0.126968
Second zero	5.250	0
Second maximum	6.239	0.038435
Third zero	7.755	0
Second minimum	8.704	-0.012472

V. FINITE n RECONSIDERED

In this section we will study the finite-n case using γ, rather than C, as the fundamental correlation function. This has the advantage that the expected short-distance singularities in C are recovered using (6), giving the correct Porod tail in the structure factor. A drawback of this approach, however, is that the exact conservation law is lost. This is because, as in the previous treatment of C, we find it necessary to truncate the equation for γ in order to solve numerically. A solution of the full nonlinear equation (5) would contain both the Porod tail and perfect conservation.

We start from Eqs. (5) and (6), which form a closed set giving the correlation function for any n. We proceed by first rewriting (5) as an explicit differential equation for γ, using the chain rule. Next we solve it numerically with appropriate boundary conditions. Finally, we use (6) to calculate C. This mimics the approach used previously for nonconserved vector fields. As before, it is convenient to rewrite the equation in terms of the scaling variable $x = r/L(t)$, with $L(t) = t^{1/4}$, and take $\alpha(t) = \alpha_m/t^{1/2}$, as in the large-$n$ solution. In this way, the final fourth-order, nonlinear differential equation for $\gamma(x)$, the normalized two-point, equal-time correlation function of the auxiliary field, is given by

$$\frac{1}{8}x\,C_\gamma\,\gamma' = \nabla_x^2\left[C_\gamma\left(\gamma'' + \frac{d-1}{x}\gamma' + \alpha_m\gamma + \frac{C_{\gamma\gamma}}{C_\gamma}(\gamma')^2\right)\right], \qquad (25)$$

where $C_\gamma, C_{\gamma\gamma}$ are the first and second derivatives of (6) and the operator ∇_x is gradient with respect to the scaling variable, i.e., $\nabla_x^2 \equiv d^2/dx^2 + [(d-1)/x]\,d/dx$, where d is the spatial dimension of the system. Explicit application of the operator ∇_x^2 in (25) generates derivatives of C up to fourth order, i.e., $C_{\gamma\gamma\gamma\gamma}$. In total the equation has 18 terms, of which seven are linear. After dividing through by C_γ, the various terms contain factors of the form $C_{\gamma\gamma}/C_\gamma$, $C_{\gamma\gamma\gamma}/C_\gamma$, and $C_{\gamma\gamma\gamma\gamma}/C_\gamma$.

In order to find the appropriate boundary conditions, we consider the nature of the solution for small and large x. The asymptotic solution is identical to the large-n case discussed in the previous sections. It contains two physical solutions, which can be combined as $\gamma(x) \sim \exp(-3x^{4/3}/16)\cos[(3\sqrt{3})x^{4/3}/16 + \phi]$, with ϕ an arbitrary phase, and two unphysical solutions, $\gamma(x) \sim \exp(3x^{4/3}/8)$ and $\gamma(x) = \text{const}$. In the small-x expansion the solution is n dependent but, as before, it has an undetermined parameter β in the quadratic term.

To keep the numerical analysis tractable, we will introduce a truncation at $O(\gamma^3)$ in the process of solving Eq. (25). We expand out (6) in powers of γ, and keep the terms that produce a differential equation with nonlinear terms up to order γ^3, i.e., we write $C_{\gamma\gamma}/C_\gamma = A_n\gamma$, $C_{\gamma\gamma\gamma}/C_\gamma = A_n$, $C_{\gamma\gamma\gamma\gamma}/C_\gamma = 0$, to the required order, with $A_n = 3/(n+2)$.

With this truncation, the small-x solution is given by

$$\gamma(x) = 1 + \beta x^2 + O(x^4)\ , \qquad (26)$$

where β is an undetermined parameter in terms of which all the higher-order coefficients in (26) can be expressed. The quadratic small-x behavior generates, via Eq. (6), the correct generalized power-law form for the tail of the structure factor.

Using the asymptotic behavior of the hypergeometric functions for $\gamma \to 1$, one can show that the leading small-x singularity in the scaling function $f(x)$ takes the form [12]

$$f_{\text{sing}}(x) = \frac{n}{2\pi}\frac{\Gamma^2[(n+1)/2]\Gamma[-n/2]}{\Gamma[(n+2)/2]}\,(2\beta x^2)^{\frac{n}{2}} \qquad (27)$$

provided n is not an even integer. The latter cases can be recovered by setting $n = 2m + \epsilon$ in the general result, letting $\epsilon \to 0$, and picking up the term of order unity (i.e., ϵ^0). This gives

$$f_{\text{sing}}(x) = -(-1)^{n/2}\frac{n}{\pi}\frac{\Gamma^2[(n+1)/2]}{\Gamma^2[(n+2)/2]}\,(2\beta x^2)^{n/2}\ln x, \qquad n \text{ even}\ . \qquad (28)$$

From these expressions the generalized Porod law [12,13] for the structure-factor scaling function can be derived: $g(q) \sim q^{-(d+n)}$ for $q \gg 1$.

In principle our solution has built in the nature of topological defects, through Eq. (6). We turn now to the approximate solution of the differential equation for γ. We proceed as before, integrating the equation of motion [truncated at $O(\gamma^3)$] forward, with the boundary conditions $\gamma(0) = 1$, $\gamma'(0) = 0$, $\gamma''(0) = 2\beta$, $\gamma'''(0) = 0$ that follow from (26). Then we eliminate the two unphysical solutions by adjusting the two unknown parameters α and β. Finally, substituting the γ solution back into Eq. (6) we determine $C(\gamma) \equiv f(x)$, the scaling function. We have solved for $n = 2$ and $n = 5$ in three dimensions. Table VI shows the eigenvalues α, β and the positions and amplitudes for the zeros and extrema of the scaling function for $n = 2$.

Figure 5(a) shows the form of the scaling function obtained with this approach, with the data of SR included. Despite the inclusion of the correct short-distance singularity, this method is much less successful at describing the data than our earlier C^3 expansion, as a comparison with Fig. 4 readily demonstrates. Presumably, the loss of the exact conservation law, evident in Fig. 5(b) for the structure-factor scaling function, is more important for the general shape of the scaling function than getting the short-distance singularity right. Somewhat surprisingly, even the small-x behavior is much better described by the C^3 truncation result displayed in Fig. 4(a). Although the structure factor in Fig. 5(b) has a tail of the correct q^{-5} form, the fit to the data in this regime is not noticeably better than Fig. 4(b).

In fact, the case $n = 2$ is the worst case for the new approximation: when one solves the problem for larger n, the solution has improved. For instance, the $n = 5$ case, presented in Fig. 6, shows that the violation of the conservation law is reduced relative to $n = 2$. All the relevant information concerning the scaling function is

TABLE VI. Information on the scaling function extracted numerically for $n = 2$ in the γ^3 approximation. The eigenvalues are $\alpha = 1.543\,505\,68$ and $\beta = -0.229\,039\,6$.

Quantity	x	$f(x)$
First zero	2.701	0
First minimum	3.706	-0.11519
Second zero	5.332	0
Second maximum	6.320	0.03488
Third zero	7.836	0
Second minimum	8.786	-0.01129

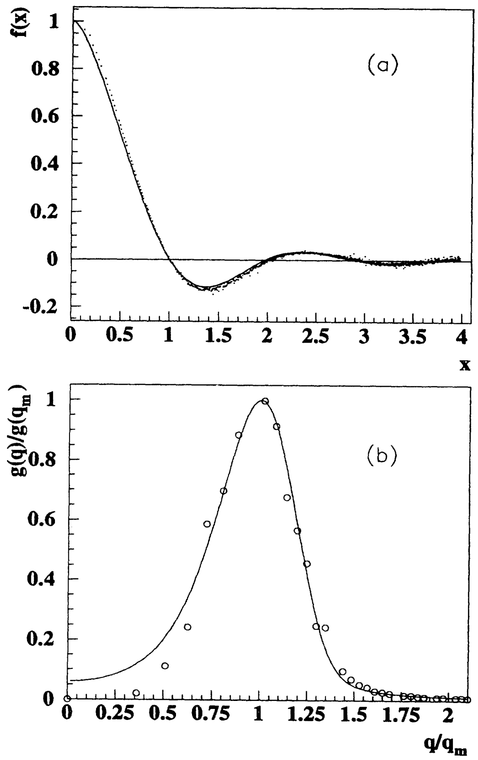

FIG. 5. (a) Scaling function for $n = 2$ with the correct small-x singularity, obtained using the γ^3 approximation as described in Sec. V. The data are from Ref. [10]. The fit is clearly not as good as Figure 4(a), even at small x. (b) The corresponding structure factor with the correct q^{-5} Porod tail.

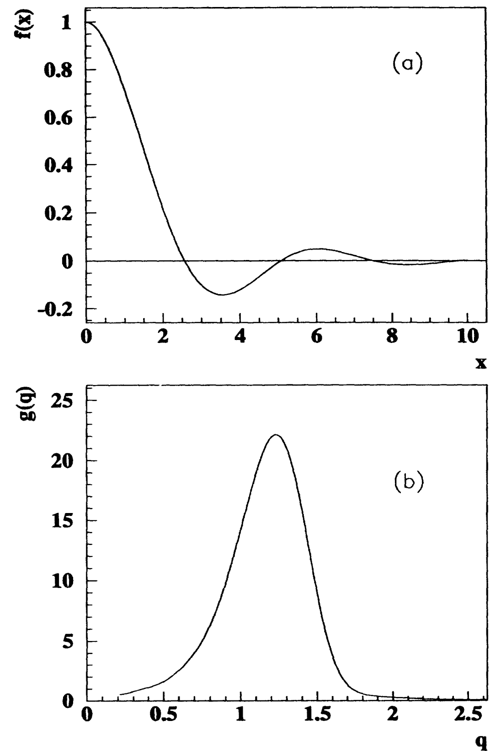

FIG. 6. (a) Scaling function for $n = 5$ within the γ^3 approximation. (b) The corresponding structure factor with the correct q^{-8} Porod tail.

detailed in Tables VI and VII. A close comparison of Table VII for $n = 5$ and Table I for the $1/n$ expansion approach with $n = 5$ shows that the two first digits, in the minimum and maximum amplitudes, are the same.

VI. SUMMARY

In summary, we have studied, in the context of the Gaussian auxiliary field approach, the dynamics of phase separation in systems with conserved vector order parameter. All our results follow standard dynamic scaling: there is no multiscaling behavior for finite n. We have solved differential equations for the scaling function using three different truncation schemes: truncation at order $1/n$, at order C^3, and at order γ^3. The structure factor for the $1/n$ truncation can be fitted very well with a quartic exponential function, motivated by the analytic solution of BH for large n. A truncation of the fundamental equation at order C^3 yields an identical equation, but with n replaced by an effective value n^*. For $n = 2$, this approach gives remarkably good agreement with the simulation results of SR. This is all the more remarkable given that the $t^{1/4}$ growth law obtained for $n = 2$ is not quite right: the correct behavior of the characteristic length scale being $L(t) \sim (t \ln t)^{1/4}$ for $n = 2$ (and $d > 2$) [7]. The C^3 truncation respects the conservation law, but does not correctly incorporate the short-distance singularities responsible for the Porod tail in the structure factor. The latter can be recovered through the γ-solution approach, at the expense of losing the conservation law (at least when we truncate the γ expansion). For $n = 2$ it is clear that respecting the conservation law is more important. For larger n, all three approaches converge.

TABLE VII. Information on the scaling function extracted numerically for $n = 5$ in the γ^3 approximation. The eigenvalues are $\alpha = 1.718\,789\,60$ and $\beta = -0.260\,360$.

Quantity	x	$f(x)$
First zero	2.561	0
First minimum	3.542	-0.14268
Second zero	5.070	0
Second maximum	6.042	0.04844
Third zero	7.481	0
Second minimum	8.420	-0.01742

ACKNOWLEDGMENTS

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