Growth kinetics for a system with a conserved order parameter

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A theory of spinodal decomposition for an ordering system with a conserved, scalar order parameter is presented. The theory supports a scaling solution for the order parameter correlation function with a growing characteristic length given by the Lifshitz-Slyozov-Wagner growth law $L \sim t^{1/3}$. The structure factor satisfies Porod's law $Q^{-(1+d)}$ at large scaled wave number Q, for spatial dimensionality d, and Q^4 at small wave number. This result for small Q is nontrivial. Comparison of the theory with numerical results shows good agreement for the order parameter scaling function. The theory builds on the post-Gaussian approximation scheme developed previously by the author [Phys. Rev. E **49**, 3717 (1994)] for the nonconserved order parameter case. It is shown that in the lowest-order post-Gaussian approximation the unphysical result in the Gaussian theory, namely that the scaling function for an auxiliary Gaussian field is negative for small wave numbers, is remedied.

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I. INTRODUCTION

Although the dynamics of the ordering process for a nonconserved order parameter (NCOP) have been well described by recent theories [1–5], a quantitative theory describing the ordering of a system with a conserved order parameter (COP) has remained elusive. In this paper, a theory of phase ordering kinetics for such systems is presented which reproduces nearly all of the qualitative features of late-stage growth. The theory developed here resolves certain technical difficulties found in earlier theories. Recent theories for treating the growth of order in unstable systems have successfully exploited the use of an auxiliary field. An important limitation imposed on the theory by assuming this field to be Gaussian is clear in the case of a conserved order parameter. It was found in Ref. 5 that the Fourier transform of the auxiliary-field autocorrelation function, which must be positive by definition, goes negative for small wave numbers. It is shown here, by going beyond the Gaussian approximation, that this autocorrelation function is rendered positive.

While it has been difficult to develop a quantitative theory for the COP case, a great deal is known about this problem from experiment, direct numerical solutions and from general arguments involving a collection of sharp interfaces. The most fundamental result is that phase-separating systems exhibit scaling [6]. In the late stage regime, the system is divided into large domains where the order parameter $\psi(\mathbf{R},t)$ takes on one of the degenerate values $\pm\psi_0$ and these domains are separated by sharp interfaces of width ξ. The dynamics depend on a single, macroscopic length, the growth law $L(t)$ which characterizes the size of the domains and the curvature of the interfaces and which grows in time. The order parameter autocorrelation function satisfies the scaling equation

$$C_{\psi,\psi}(\mathbf{R},t) \equiv \langle \psi(\mathbf{R},t)\psi(0,t)\rangle = \psi_0^2 F(x) , \tag{1.1}$$

where $x \equiv R/L(t)$ and $x \gg \xi/L(t)$. The structure factor is the Fourier transform of $C_{\psi,\psi}(\mathbf{R},t)$ which satisfies

$$C_{\psi,\psi}(\mathbf{q},t) = L^d \psi_0^2 \tilde{F}(Q) , \tag{1.2}$$

where $Q \equiv qL$ is a scaled wave number and d is the dimension. It has been established in a variety of ways that $L(t)$ (Refs. [7–9]) is given by the Lifshitz-Slyosov-Wagner (LSW) result $L \sim t^{1/3}$.

There are several other important features which a theory of spinodal decomposition should include.

(1) Scattering from a collection of sharp interfaces (width $\xi \ll L$) obeys Porod's law,

$$\tilde{F}(Q) \sim Q^{-(d+1)} \tag{1.3}$$

for large Q [10]. Equivalently, in coordinate space this means that the first correction is nonanalytic in x and has the general expansion

$$F(x) = 1 - \alpha x(1 + \beta_2 x + \beta_3 x^2 + \cdots) , \tag{1.4}$$

for small scaled distances x.

(2) Tomita [11] showed, assuming that interfaces are sufficiently smooth, that the coefficients of even powers of x vanish, $\beta_{\text{even}} = 0$ in Eq. (1.4).

(3) The small Q behavior of the structure factor is given by

$$\tilde{F} \sim Q^4 . \tag{1.5}$$

This last result is supported by simulations [12] and phenomenological arguments [13], but no previous dynamical theory could account for this feature. Indeed, the correlation functions derived below exhibits all the features mentioned above except for the Tomita sum rule, which is also the most difficult to verify empirically.

Essentially all of the current theories for the growth of order in an unstable systems assume the existence of an underlying Gaussian auxiliary field. In previous work [2,3], this variable $m(\mathbf{R},t)$ has the physical interpretation

that its magnitude gives the distance from $\mathbf{R}$ to the nearest interface. It is assumed that the order parameter can be expressed as a sum of an ordering field σ, which is a local functional of m, and a field ϕ which can be ignored in the scaling regime. These theories have had many successes and the basic development has been pushed very far. In this paper, it is shown how the method developed by the author for the NCOP case can be extended to treat the conserved order parameter case and explain essentially all of the features outlined above. In the course of this work, it should become clear why the COP case is so difficult. The appropriate theory in this case is not a straight-forward generalization of the method which has been successful in treating the NCOP case. While the most direct implementation of the basic method [14] is analytically appealing and elegant, it is wrong in a number of important ways. In the most direct application of the method developed in Ref. 2, one does obtain scaling, universality, and Porod's law—a substantial accomplishment. There are, however, serious problems.

(1) Instead of the LSW growth law, one obtains the result $L \sim t^{1/4}$ which is characteristic of surface diffusion.

(2) For small scaled wave numbers Q the structure factor goes as Q^2 rather [15] than the observed Q^4.

(3) The structure factor for the Gaussian auxiliary field goes negative for small wave numbers. This unphysical result caused Yeung, Oono, and Shiriozaki [5] to call the entire theoretical development into question. Concern is justified since this structure factor is related to the basic probability distribution governing the theory and its lack of positivity calls into question the stability of the solutions obtained.

(4) In the COP case the Tomita sum rule is not, unlike the NCOP case, naturally satisfied in the theory. Indeed it appears to be violated by the theory in a substantial way.

(5) Since ψ is conserved, one has for a general field G, which is not conserved, the result

$$\langle \psi(\mathbf{q}) G(-\mathbf{q}) \rangle \approx q^2 \tag{1.6}$$

for small wave number $\mathbf{q}$. As will be shown below, it does not appear to be possible to obtain this result within the Gaussian approximation.

The resolution of the first three of these problems turns out to require a rather substantial generalization of the theory developed in Ref. [2]. A key first step is to understand the important role of the diffusion field u of $O(1/L)$ relative to the ordering field σ. It was suggested in Ref. [14] that this inclusion could resolve the problem with the growth law and give the LSW result. The way it was treated there, however, was too *ad hoc* to remedy problem (2). The resolution of problems 1 and 2 comes from the proper treatment of the diffusion field. As discussed in detail in Sec. VI D, problem 3 can only be dealt with by going beyond the standard Gaussian methods. In Ref. [3] the author has shown how to introduce such approximations in general, and, in particular, how the lowest-order correction can improve the theory when compared with the Gaussian theory. Similarly, problem 5 above can be addressed only by going beyond the Gaussian approximation.

In the NCOP case, it was shown how, by simply including the first logical correction to the Gaussian case, one can qualitatively change some aspects of the zeroth-order solution. In particular, it was shown how the improved theory can explain the recent numerical results of Blundell, Bray, and Suttler (BBS) (Ref. [16]), which are in qualitative disagreement with Gaussian theories. They recently proposed an absolute test for theories of phase-ordering dynamics. They considered an unstable system with an order parameter $\psi(1)=\psi(\mathbf{R}_1,t_1)$, which has an ordered value $\lim_{t_1\to\infty}\psi^2(1)=\psi_0^2$. They then point out, based on direct numerical evaluation, that a plot of the quantity

$$C_{\psi^2}(12)=\frac{\langle[\psi_0^2-\psi^2(1)][\psi_0^2-\psi^2(2)]\rangle}{\langle[\psi_0^2-\psi^2(1)]\rangle\langle[\psi_0^2-\psi^2(2)]\rangle}-1 \tag{1.7}$$

versus the square of the order parameter correlation function $C_{\psi,\psi}(12)$ has a qualitatively different behavior for small C_{ψ^2} than that predicted by existing "Gaussian" theories which give

$$C_{\psi^2}=\frac{\pi^2}{8}[C_{\psi,\psi}/\psi_0^2]^2 . \tag{1.8}$$

The numerical work by BBS indicates that C_{ψ^2} goes to zero much faster than $C_{\psi,\psi}^2$ for small $C_{\psi,\psi}$. It seems clear that one must go beyond the Gaussian approximation to obtain this result. In Ref. [3] a general theory was developed where the Gaussian approximation serves as an accurate zeroth-order approximation. More particularly, it is shown that by including the first non-Gaussian correction, the result of BBS described above is obtained in a nontrivial manner. This gives one encouragement to go on and apply these same ideas to the COP case.

In the next section, we define the problem and then move on in Sec. III to a discussion of the ideas behind the structure of the theory. These ideas are then implemented in successively more sophisticated approximations in Secs. IV, V, and VI. In Sec. IV the naive Gaussian approximation (NGA) is discussed. In this approximation, the diffusive field u is ignored and the auxiliary field m is assumed to be a Gaussian variable. In the Gaussian diffusion approximation (GDA) the diffusion field u is introduced, but again m is treated as a Gaussian field. Finally, in Sec. VI, in the lowest-order post-Gaussian approximation (PGA), the diffusion field is included and m is treated beyond the Gaussian approximation.

II. PROBLEM STATEMENT

As usual it is assumed that the dynamics of spinodal decomposition in its simplest form can be described by a Langevin equation of the time-dependent Ginzburg-Landau (TDGL) or Cahn-Hilliard type which drives the evolution of a scalar order parameter $\psi(\mathbf{R},t)$:

$$\frac{\partial\psi}{\partial t}=D_0\nabla^2[V'(\psi)-\nabla^2\psi]+\eta . \tag{2.1}$$

The noise η in Eq. (2.1) is assumed to be Gaussian with variance

$$\langle \eta(1)\eta(2)\rangle = 2k_B T(-D_0\nabla_1^2)\delta(12) , \tag{2.2}$$

where T is the temperature of the driving bath and, for example, 1 is the short-hand notation for $(\mathbf{R}_1,t_1)$ and

$$\delta(12)=\delta(\mathbf{R}_1-\mathbf{R}_2)\delta(t_1-t_2) . \tag{2.3}$$

In Eq. (2.1) $V(\psi)$ is a degenerate, double-welled potential with minima at $\pm\psi_0$ and D_0 is a bare diffusion coefficient. The conservation law is enforced by the Laplacian acting on the right-hand side of Eq. (2.1). The physical situation of interest corresponds to a rapid temperature quench at time t_0 from an initial disordered state to a final bath temperature T below the ordering temperature. One can neglect the noise in Eq. (2.1) with the expectation that thermal fluctuations are irrelevant for late-time ordering. Stochasticity is introduced via random initial conditions characterized by (Gaussian) initial conditions with zero average and variance

$$\langle \psi_0(\mathbf{R})\psi_0(\mathbf{R}')\rangle = \epsilon_0\delta_{\mathbf{R},\mathbf{R}'} , \tag{2.4}$$

where $\psi_0(\mathbf{R})=\psi(\mathbf{R},t_0)$. Thus, the initial state is assumed to be completely disordered. The analysis is restricted here, for simplicity, to the high symmetry case of a critical quench where the average of the order parameter vanishes

$$\langle \psi(1)\rangle = 0 . \tag{2.5}$$

The important case of an off-critical quench $[\langle \psi(\mathbf{R},0)\rangle \neq 0]$ will be considered elsewhere.

It will be useful in the discussion below to rewrite Eq. (2.1) in the form

$$\Lambda(1)\psi(1)=D_0\nabla_1^2 V'(\psi(1))+\eta(1) , \tag{2.6}$$

where

$$\Lambda(1)=\frac{\partial}{\partial t_1}+D_0\nabla_1^4 . \tag{2.7}$$

III. STRUCTURE OF THEORY

A. Review of original method

1. Separation of fields

The original theory developed for the NCOP case begins with the separation of the order parameter into two pieces [17]:

$$\psi(\mathbf{R},t)=\sigma(m(\mathbf{R},t))+\phi(\mathbf{R},t) , \tag{3.1}$$

where σ is a local function of a new auxiliary field m which governs the domain structures and ϕ, roughly speaking, represents the fluctuations within ordered domains. The introduction of the ordering field σ and the auxiliary field m involve several technical points which are often glossed over. A full discussion is given in Refs. [3,18]. The main point is that $\sigma(1)$ and $m(1)$ can be introduced into the theory rather generally and the field $\phi(1)$ will not contribute to the late stage ordering if

(1) The quantity

$$q_0^2(1)=\langle V''(\sigma(1))\rangle_\sigma \tag{3.2}$$

becomes positive as the system orders.

(2) The quantity

$$B(1)=\Lambda(1)\sigma(1)-D_0\nabla_1^2 V'(\sigma(1)) \tag{3.3}$$

is small in the scaling regime.

These conditions ensure that $\phi(1)$ remains small in amplitude and is stable (decaying) at late times. Once one understands the conditions under which the field m can be introduced and that the field ϕ serves as a perturbation at long times, one must, as pointed out in some detail in Ref. [17], introduce a probability distribution $P[m]$, which governs the m fields. It is the average over $P[m]$ which appears in the definition of $q_0^2(1)$ and feeds back on conditions (1) and (2) above. Thus, one must choose $P[m]$ consistent with the requirement that B be *small*. At the formal level, the simplest choice [19] guaranteeing that $B(1)$ be small is to choose $B(1)=0$. This is equivalent to assuming that σ satisfy the original equation of motion with $\psi\to\sigma$ for a quench to zero temperature where the noise can be set to zero. This choice implicitly determines the underlying probability distribution $P[m]$ governing the variable m. The $P[m]$ associated with the very rigid condition $B(1)=0$ will be very far from a Gaussian and the associated problem will be as difficult as the original problem in terms of ψ. The alternative is to balance the need to have $B(1)$ small and to have $P[m]$ be near a Gaussian and assume that weighted averages of $B(1)$ are zero. Since $\langle B(1)\rangle_0=0$ by symmetry, where $\langle\ \rangle_0$ indicates an average over a Gaussian $P[m]$, the simplest nonzero average is given by

$$\langle B(1)\sigma(2)\rangle_0 = 0 . \tag{3.4}$$

Assuming that $P[m]$ is a Gaussian distribution, Eq. (3.4) is sufficient to determine the variance $\langle m(1)m(2)\rangle_0$ and all other averages over m.

It was found in Ref. [2] that these conditions are sufficient to make the σ variable order. If the σ variable orders then σ^2 approaches its uniform value ψ_0^2, $q_0^2(1)$ is positive at late times, and $\Lambda(1)\sigma(1)$ and $V'(\sigma(1))$ approach zero in the long-time limit. Thus while $B(1)$ is not identically zero, it will be small at late times. In the scaling regime one estimates

$$B(1)\approx 1/t\approx 1/L^3 . \tag{3.5}$$

2. The auxiliary field m

The introduction of the auxiliary field m represents a key step in the analysis. One expects that it is smoother than ψ, but its zeros coincide with those of ψ and mark the position of the interfaces. The field $m(\mathbf{R},t)$ has the physical interpretation that its magnitude gives the distance from $\mathbf{R}$ to the nearest interface. Then near an interface $m\approx 0$, but well away from an interface of thickness ξ, $m\gg\xi$, one has

$$\sigma[m]=\mathrm{sgn}(m)\psi_0 \tag{3.6}$$

where ψ_0 is the equilibrium magnitude of the average

value of the order parameter. Thus while m will smoothly vary through an interface, σ will show a sharp behavior. This physical picture can be realized by assuming [2] that $\sigma(m)$ satisfies the classical equation for an equilibrium interface:

$$\tfrac{1}{2}\sigma_2(m)=V'(\sigma(m)) , \tag{3.7}$$

with m the associated coordinate. In Eq. (3.7) the factor $\frac{1}{2}$ is inserted for convenience, the notation

$$\sigma_n(m)\equiv\partial^n\sigma(m)/\partial m^n \tag{3.8}$$

is introduced and the boundary conditions are

$$\lim_{m\to\pm\infty}\sigma=\pm\psi_0 . \tag{3.9}$$

This choice for σ guarantees that the system orders with the appropriate values of ψ_0. It should be clear from the physics of the situation that at long times the fields m and ϕ are essentially independent and should be viewed as fluctuating in separate function spaces. Since the distance between interfaces grows with time we expect

$$S_0(t)=\langle[m(\mathbf{R},t)]^2\rangle \tag{3.10}$$

$$\sim L^2(t) . \tag{3.11}$$

3. *Naive theory*

In the most elementary version of the theory, for both the NCOP and COP cases, it is assumed that m is a Gaussian field and the average of the equation of motion in the form

$$\langle B(1)\sigma(2)\rangle_0=0 \tag{3.12}$$

determines the variance

$$C_0(12)=\langle m(1)m(2)\rangle_0 \tag{3.13}$$

which, because m is a Gaussian variable, also determines

$$C_{\sigma,\sigma}(12)=\langle\sigma(1)\sigma(2)\rangle_0 . \tag{3.14}$$

Essentially any quantity can then be evaluated in terms of C_0. We analyze the consequences of this theory in detail below in Sec. IV.

B. Diffusion field

As explained in the introduction and in more detail below, the naive theory fails in several ways. The formally most obvious place where the theory may be questioned concerns the Gaussian approximation for the probability distribution $P[m]$. This point is discussed in the next section. Here, the physically important improvement in the theory associated with the inclusion of a diffusion field will be discussed [20].

In the conserved case there is a nonequilibrium current which flows across ordered regions and couples distant interfaces. If we look at a perturbation $u(\mathbf{R},t)$ [21] in a region ordered with $\psi=+\psi_0$,

$$\psi=\psi_0-u , \tag{3.15}$$

and linearize the equation of motion, Eq. (2.1), in u we obtain

$$\frac{\partial u}{\partial t}=D_0\nabla^2[V''(\psi_0)u-\nabla^2u] , \tag{3.16}$$

where we ignore the noise. In the scaling regime, where $\nabla\approx L^{-1}$, and $\partial/\partial t_1\approx L^{-3}$, this reduces to the familiar result $\nabla^2u=0$ away from the interfaces. More generally, since $V''(\psi_0)>0$, one has a diffusive dynamics. In an A-B alloy, for instance, u includes the current of $A(B)$ atoms through regions of ordered $B(A)$ phase. The interfaces are the source of u with a contribution proportional to the local curvature. Because the curvature depends only on the length scale L, we expect $u\sim O(1/L)$. With the goal of describing a set of ordered domains with the superposed diffusive field coupling the interfaces, we write [22] $\psi=\sigma(m)-u$ which we insert in Eq. (2.1) and expand in powers of u to obtain

$$\frac{\partial\sigma}{\partial t}=D_0\nabla^2[-q_0^2u+\tfrac{1}{2}\sigma_2-\nabla^2\sigma+O(u^2)] , \tag{3.17}$$

where

$$q_0^2\equiv\langle V''(\sigma)\rangle=V''(\psi_0)+O(1/L) , \tag{3.18}$$

and the average is over m. We will see below that only the u term on the right-hand side of Eq. (3.17) will contribute to the scaling properties of the system. (Loosely speaking, the terms σ_2 and $\nabla^2\sigma$ enforce the shape of the interfaces and do not contribute to the scaling behavior.) Counting powers of L immediately gives us $[t]\sim[L^3]$, $n=\frac{1}{3}$.

The key step in our development is to choose a constitutive relationship for u in terms of the fields we have available: $\sigma(m)$ and m. The field should be a scalar, conserved in the bulk, odd in m, and of $O(1/L)$. It should be recognized that taking $u\approx O(L^{-1})$ breaks a symmetry in the theory associated with the result that a general correlation function $C_{A,B}(12)$ in the scaling regime is given in terms of even powers of L^{-1}.

The condition that u be conserved,

$$\int d^dR\,u(\mathbf{R},t)=0 , \tag{3.19}$$

is closely related to the requirement that $\tilde{F}(Q)\approx Q^4$ for small Q. These considerations lead to the general form

$$u(\mathbf{R},t)=\frac{u_0}{L}\sigma(\mathbf{R},t)+\nabla^2u_1(\mathbf{R},t) . \tag{3.20}$$

It is worth noting that while σ is conserved $\sigma(\nabla m)^2$, for example, is not. Thus, it is not an option to choose u_0 as a function of m. Since the Laplacian is of $O(L^{-2})$, u_1 must be of $O(L)$. One has the general expansion [23]

$$u_1=\lambda m[1+\lambda_3(\nabla m)^2+\lambda_5(\nabla m)^4+\cdots] . \tag{3.21}$$

While one could take the λ's to be a function of σ^2, this would make no difference in the scaling regime where one can replace σ^2 with ψ_0^2. In this paper, only the simplest assumption

$$u=\frac{u_0}{L}\sigma+\lambda\nabla^2 m \tag{3.22}$$

is explored. Taking Eq. (3.22) as our ansatz for u, our expression for ψ becomes

$$\tilde{\psi}=\sigma(m)\left[1-\frac{u_0}{L}\right]-\lambda\nabla^2 m \ . \tag{3.23}$$

The two additional terms can each be given a natural interpretation. Near an interface, ∇m is normal to the interface and of constant magnitude, so $\nabla^2 m$ is a measure of the local interfacial curvature. The u_0 term diminishes ψ everywhere by an amount proportional to the mean interfacial curvature.

A key element in the development here is that ψ now depends on $\nabla^2 m$ as well as m and the quantity $B(1)$, defined by Eq. (3.3), must be generalized by replacing $\sigma\rightarrow\tilde{\psi}$ to obtain

$$\tilde{B}(1)=\Lambda(1)\tilde{\psi}(1)-D_0\nabla_1^2 V'(\tilde{\psi}(1)) \ . \tag{3.24}$$

C. General distribution function for m

How can one generalize previous work and gain some control over the probability distribution governing the variable m? Again, the idea is to *minimize* $\tilde{B}(1)$ while still having a near Gaussian distribution for m. One can begin by assuming that m is governed by a general probability distribution $P[m]$ given by an expansion in terms of generalized Hermite polynomials:

$$P[m]=e^{-K_0[m]}\sum_{n=0}^{\infty}A_n(12\ldots n)H_n(12\ldots n) \ , \tag{3.25}$$

where integrals over repeated indices are implied and the generalized Hermite *polynomials* are defined by the functional derivatives

$$H_n(12\ldots n)=(-1)^n e^{K_0[m]}\times\frac{\delta^n}{\delta m(1)\delta m(2)\cdots\delta m(n)}e^{-K_0[m]} \ , \tag{3.26}$$

where

$$K_0[m]=\tfrac{1}{2}\int d1\,d2\,m(1)C_0^{-1}(12)m(2) \tag{3.27}$$

and $C_0^{-1}(12)$ is the matrix inverse of $C_0(12)$

$$\int d3\,C_0^{-1}(13)C_0(32)=\delta(12) \ . \tag{3.28}$$

Various averages can then be worked out in terms of Gaussian averages $\langle\ \rangle_0$. For example the average of a one-point quantity is given by

$$\langle\phi(m(1))\rangle=\sum_{n=0}^{\infty}A_n^{(0)}(1)\langle\phi_n(1)\rangle_0 \ , \tag{3.29}$$

where we introduce the convenient notation

$$\phi_n(m(1))\equiv\frac{d^n}{dm^n(1)}\phi(m(1)) \tag{3.30}$$

and

$$A_n^{(0)}(1)\equiv A_n(11\ldots1) \ . \tag{3.31}$$

A general two-point average can be written in the form

$$\langle\phi(1)\chi(2)\rangle=\sum_{n=0}^{\infty}\sum_{s=0}^{n}\frac{n!}{s!(n-s)!}A_{n;s}(1,2)\langle\phi_{n-s}(1)\chi_s(2)\rangle_0$$
$$=\langle\phi(1)\chi(2)\rangle_0+A_2(11)\langle\phi_2(1)\chi(2)\rangle_0+2A_2(12)\langle\phi_1(1)\chi_1(2)\rangle_0+A_2(22)\langle\phi(1)\chi_2(2)\rangle_0+\cdots \ . \tag{3.32}$$

Here we have also introduced the notation $A_{n;s}(1;2)$ to indicate that A_n has s arguments equal to 2 and $n-s$ arguments equal to 1. It is assumed that we have a symmetric quench such that all A_n with odd n vanish. For $n=2$ there is an additional (beyond C_0) independent function $A_2(12)$ for determining all two-point functions.

The idea is to use a sequence of constraints to determine the coefficients A_n. Since ultimately one requires that the quantity $\tilde{B}(1)$ be small, one can choose the coefficients A_n, up to order n, by enforcing the constraints

$$\langle\tilde{B}(1)\sigma(2)\rangle=0 \ , \tag{3.33}$$

$$\langle\tilde{B}(1)\sigma(2)\sigma(3)\sigma(4)\rangle=0 \ , \tag{3.34}$$

etc., up to level n. In principle, as n increases, one might suppose that the theory enforces the condition that $\tilde{B}(1)$ be small more effectively. In the work here, we will look at the lowest-order versions of this theory.

IV. NAIVE GAUSSIAN APPROXIMATION

In this section, we explore the naive theory formally presented in Sec. III A 3.

A. Scaling equation of motion

In the scaling limit in the case of equal times ($t_1=t_2=t$) one finds, to leading order in L^{-1}, with $\psi(1)=\sigma(m(1))$ and the m dependence of σ satisfying Eq. (3.7),

$$C_{\psi,\psi}(12)=C_{\sigma,\sigma}(12)=\psi_0^2 F(x) \ , \tag{4.1}$$

where $x=|\mathbf{R}_1-\mathbf{R}_2|/L$ and $L^2(t)\equiv\pi S_0(t)$. Since the field m is a Gaussian variable the scaling function can be expressed back in terms of the variance of the field m:

$$F(x)=\frac{2}{\pi}\sin^{-1}f(x)\ , \tag{4.2}$$

where, returning to a more general parametrization,

$$f(12)=C_0(12)/S_0(t)\ . \tag{4.3}$$

In the scaling limit f is only a function of x. The quantity

$$\gamma(12)=1/\sqrt{1-f^2(12)} \tag{4.4}$$

also naturally enters the analysis. In evaluating the averages in Eq. (3.12) one needs, for example, the result valid in the scaling regime,

$$\begin{aligned}C_{\sigma_2,\sigma}(\mathbf{R},t)&=-\frac{2\psi_0^2}{L^2}f(x)\gamma(x)\\&=-\frac{2\psi_0^2}{L^2}\tan\left[\frac{\pi}{2}F\right]\ .\end{aligned} \tag{4.5}$$

Using this result in Eq. (3.12) and introducing scaled variables, one obtains

$$\mu_0\mathbf{x}\cdot\nabla F(x)=\nabla^2\left[\tan\left[\frac{\pi}{2}F\right]+\nabla^2F\right]\ , \tag{4.6}$$

where $2D_0\mu_0=L^3\dot{L}$. Assuming that μ_0 is a constant immediately gives the surface diffusion growth law $L(t)\approx t^{1/4}$. The key ideas in finding the solution of the scaling equation, Eq. (4.6), is discussed in some detail in Refs. [2,14].

B. Analytic results

1. Short distances

The key points involved in solving Eq. (4.6) follow from a study of its short- and large-distance solutions. For short scaled distances F is of the form given by Eq. (1.4). The coefficient in the term of $O(x)$, corresponding to Porod's law, is given by

$$\alpha=\left[\frac{2}{\pi(d-1)}\right]^{1/2}\ , \tag{4.7}$$

which is the same as for the NCOP case, β_3 is given in Ref. [14] and the β_{even} are proportional to β_2 which is undetermined from the short-distance behavior.

2. Long distances

For large x, where F is small, one can again solve Eq. (4.6) analytically. There are a number of solutions including a growing exponential solution, an algebraically decaying solution and the physically acceptable damped oscillatory solution given by

$$\begin{aligned}F=F_0x^{-2d/3}&\exp\left[-\tfrac{3}{8}\mu_0^{1/3}\left[x^{4/3}-\frac{\pi}{3\mu_0^{2/3}}x^{2/3}\right]\right]\\&\times\cos\left[\sqrt{3}\tfrac{3}{8}\mu_0^{1/3}\left[x^{4/3}+\frac{\pi}{3\mu_0^{2/3}}x^{2/3}+\phi\right]\right]\ ,\end{aligned} \tag{4.8}$$

where F_0 and ϕ are constants.

3. The eigenvalue problem

The matching of the short distance and the physically acceptable long-distance behavior can only be achieved for selected values for μ_0 and β_2. One of the important characteristics of the method developed in Ref. [2], and in subsequent work, is the introduction of a nonlinear eigenvalue problem. This is the mechanism which enforces universality so that the scaling function F depends only on d. In the NCOP case, a parameter analogous to μ_0 is selected. In the COP case one has the additional parameter β_2. This can easily be seen by integrating Eq. (4.6) using the Green's function for the Laplacian (see Ref. [14]) and using the result that F is isotropic in $\mathbf{x}$. One then obtains for $(d>2)$

$$\nabla^2F+\tan\left[\frac{\pi}{2}F\right]=\frac{\mu_0}{d-2}\left[\frac{dI_d(x)}{x^{d-2}}-2[I_2(x)-I_2(\infty)]\right] \tag{4.9}$$

where

$$I_d(x)=\int_0^x dy\,y^{d-1}F(y)\ . \tag{4.10}$$

Inserting the short-distance expansion Eq. (1.4) for F one easily finds

$$-\beta_2\alpha(3d-1)=\frac{2\mu_0}{d-2}I_2(\infty) \tag{4.11}$$

and we must vary $I_2(\infty)$ (and β_2) to find the physical solution. Since the physical solution selects a nonzero β_2, one finds, for nontrivial reasons, that this theory does not satisfy the Tomita sum rule. This is unlike the NCOP case where the Tomita sum rule is satisfied naturally within the theory. One therefore has a nonlinear eigenvalue problem with $\mu_0=0.337\,596$, $\beta_2=-0.0778$ for $d=2$, while $\mu_0=0.175\,171$ and $\beta_2=-0.0356$ for $d=3$.

4. Spatial moments

One can gain insight into the quality of this solution by looking at the moments of the scaling function

$$W_p=\int d^dx x^pF(x)\ . \tag{4.12}$$

The lower-order moments can be evaluated analytically by multiplying Eq. (4.6) by x^p, p an even integer, and integrating over all $\mathbf{x}$ to obtain

$$W_0=0\ , \tag{4.13}$$

which is a statement of the conservation law, and

$$W_2=\frac{-2d}{\mu_0(d+2)}\int d^dx\,\tan\left[\frac{\pi}{2}F(x)\right]. \tag{4.14}$$

These results should be interpreted in the following light. It can be shown numerically that

$$W_{\sin}\equiv\int d^dx\,\sin\left[\frac{\pi}{2}F(x)\right] \tag{4.15}$$

is negative, while

$$W_{\tan}\equiv\int d^dx\,\tan\left[\frac{\pi}{2}F(x)\right] \tag{4.16}$$

is positive. One can understand these results qualitatively by expanding the trigonometric functions inside the integrals and using the conservation law, $W_0=0$, to obtain

$$W_{\sin}=-\frac{\pi^3}{48}\int d^dxF^3(x)+\cdots, \tag{4.17}$$

$$W_{\tan}=\frac{\pi^3}{24}\int d^dxF^3(x)+\cdots. \tag{4.18}$$

Since W_0 is zero there must be cancellation between the positive and negative regions in $F(x)$. Since F^3 will have more weight in the small x regime, where it is positive, than in the smaller amplitude regime where F is negative, we expect

$$\int d^dxF^3(x)>0 \tag{4.19}$$

and

$$W_{\sin}<0 \tag{4.20}$$

and

$$W_{\tan}>0\,. \tag{4.21}$$

The condition $W_{\tan}>0$ gives $W_2<0$. This guarantees that

$$\begin{aligned}\tilde{F}(Q)&=\int d^dxe^{i\mathbf{Q}\cdot\mathbf{x}}F(x)\\&=-\frac{Q^2}{d}W_2+O(Q^4)\end{aligned} \tag{4.22}$$

is positive for small scaled wave numbers and goes as Q^2 for small Q. The result $W_{\sin}<0$, however, gives

$$\begin{aligned}\tilde{f}(Q)&=\int d^dxe^{i\mathbf{Q}\cdot\mathbf{x}}f(x)\\&=\int d^dxe^{i\mathbf{Q}\cdot\mathbf{x}}\sin\left[\frac{\pi}{2}F(x)\right]\\&=-\frac{Q^2}{d}W_{\sin}<0\end{aligned} \tag{4.23}$$

for small Q. This is the unphysical result discussed by Yeung, Oono, and Shinozaki [5] and appears to be a general result for Gaussian theories.

V. GAUSSIAN DIFFUSION APPROXIMATION

A. Scaling equation of motion

We turn now to the model which includes the diffusion field given by Eq. (3.22) but where m is still treated as a Gaussian variable. This will be called the Gaussian diffusion approximation (GDA). This theory resolves many of the problems associated with the naive theory. In Sec. III B, we argued heuristically that this theory leads to the LSW growth law $L\approx t^{1/3}$. We go through the analysis here more carefully. We evaluate

$$\langle\tilde{B}(1)\sigma(2)\rangle_0=0 \tag{5.1}$$

for the case of equal times, $t_1=t_2=t>0$, in the scaling regime (where $R=|\mathbf{R}_1-\mathbf{R}_2|$, and $L\gg\xi$) with $\tilde{B}(1)$ given by Eq. (3.24) and $\tilde{\psi}$ given by Eq. (3.23). This calculation must be carried out with care. The first step is to show, dropping terms of $O(L^{-4})$ and higher that Eq. (5.1) reduces to

$$\frac{\partial}{\partial t}C_{\sigma,\sigma}(\mathbf{R},t)=2D_0\nabla_R^2\Sigma(\mathbf{R},t)\,, \tag{5.2}$$

where

$$\Sigma(\mathbf{R},t)=W(\mathbf{R},t)-\nabla_R^2C_{\tilde{\psi},\sigma}(\mathbf{R},t)\,, \tag{5.3}$$

$$W(\mathbf{R},t)=\langle V'(\tilde{\psi}(\mathbf{R},t))\sigma(\mathbf{0},t)\rangle_0\,, \tag{5.4}$$

and the notation

$$C_{A,B}(\mathbf{R},t)=\langle A(\mathbf{R},t)B(0,t)\rangle_0 \tag{5.5}$$

is introduced. We will now show that the leading order contribution to Σ is of $O(L^{-1})$. Therefore, we can drop terms of higher order.

Consider first the second term in Eq. (5.3). One easily finds that

$$C_{\tilde{\psi},\sigma}(\mathbf{R},t)=\left[1-\frac{u_0}{L}\right]C_{\sigma,\sigma}(\mathbf{R},t)-\lambda\nabla_R^2C_{m,\sigma}(\mathbf{R},t)\,. \tag{5.6}$$

Since $C_{\sigma,\sigma}\approx O(1)$, $C_{m,\sigma}\approx O(L)$,

$$-\nabla_R^2C_{\tilde{\psi},\sigma}(\mathbf{R},t)\approx O(L^{-2}) \tag{5.7}$$

and to leading order

$$\Sigma(\mathbf{R},t)=W(\mathbf{R},t)\,. \tag{5.8}$$

The more complicated quantity, $W(\mathbf{R},t)$, can be treated by expanding the derivative of the potential in a power series in u

$$\begin{aligned}V'(\psi)&=V'(\sigma-u)\\&=\tfrac{1}{2}\sigma_2+\sum_{l=1}^{\infty}\frac{(-u)^l}{l!}V^{(l+1)}(\sigma)\,,\end{aligned} \tag{5.9}$$

where, in the first term, Eq. (3.7) has been used. Inserting Eq. (5.9) into W, given by Eq. (5.4), one obtains

$$W(\mathbf{R},t)=\tfrac{1}{2}C_{\sigma_2,\sigma}(\mathbf{R},t)+\sum_{l=1}^{\infty}W^{(l)}(\mathbf{R},t)\,, \tag{5.10}$$

where

$$W^{l}(\mathbf{R},t)=\frac{(-1)^{l}}{l!}\langle u^{l}(\mathbf{R},t)V^{(l+1)}(\sigma(\mathbf{R},t))\sigma(0,t)\rangle_{0} . \tag{5.11}$$

A key result used in the evaluation of the $W^{(l)}$ is the recursion relation obeyed by the matrix elements:

$$\begin{aligned}\mathcal{M}^{(s)}_{A,B}(12)&=\langle A(1)[\nabla^{2}m(1)]^{s}B(2)\rangle_{0}\\&=(s-1)S_{0}^{(4)}\mathcal{M}^{(s-2)}_{A,B}-S_{0}^{(2)}\mathcal{M}^{(s-1)}_{A_{1},B}\\&\quad+\nabla_{1}^{2}C_{0}(12)\mathcal{M}^{(s-1)}_{A,B_{1}} ,\end{aligned} \tag{5.12}$$

where the useful notation

$$S_{0}^{(2s)}=\langle(\nabla^{s}m)^{2}\rangle_{0} \tag{5.13}$$

is introduced and A_1, for example, indicates the derivative of $A[m(1)]$ with respect to $m(1)$. Repeated use of this result, together with the fact that $C_{A,B}\approx O(L^{-2})$ if either A or B contains derivatives of σ, allows one to show that the leading order contributions to W are of $O(L^{-1})$. Note, for example, that the contribution $\frac{1}{2}C_{\sigma_2,\sigma}$ in Eq. (5.10), which contributed to the scaling equation in the naive theory, does not contribute in this case because, as given by Eq. (4.5), $C_{\sigma_2,\sigma}\approx O(L^{-2})$. The only term of $O(L^{-1})$ contributing to W is

$$W^{(1)}(\mathbf{R},t)=-\frac{u_{0}q_{0}^{2}}{L}C_{\sigma,\sigma}(\mathbf{R},t)-\lambda q_{0}^{2}\nabla_{R}^{2}C_{m,\sigma}(\mathbf{R},t) \tag{5.14}$$

and all other $W^{(l)}(\mathbf{R},t)$ are of higher order in L^{-1} in the scaling regime. In this analysis it is useful to introduce the general notation

$$\Delta_{s}\psi_{0}^{2}=\lim_{|x|\to\infty}\sigma(x)V^{(2s+1)}(\sigma(x)) , \tag{5.15}$$

$$q_{s-1}^{2}=\lim_{|x|\to\infty}V^{(2s)}(\sigma(x)) . \tag{5.16}$$

It has been assumed in this development that

$$S_{0}^{(4)}\approx O(L^{-2}) \tag{5.17}$$

and

$$S_{0}^{(6)}\approx O(L^{-1}) . \tag{5.18}$$

It may be possible to find solutions where $S_0^{(4)}\approx O(L^{-1})$. Such solutions are more complex in nature and require a detailed study of the nonuniversal short-distance behavior in the system. The detailed interpretation of the parameters λ and u_0 in this case will depend on the behavior of $S_0^{(4)}$. Since these results do not influence the scaling behavior of the system, we make the simpler assumption given by Eq. (5.17). Inserting these results for W back into the equation of motion, we obtain

$$\frac{1}{2}\frac{\partial}{\partial t}C_{\sigma,\sigma}=-D_{0}q_{0}^{2}\nabla^{2}\left[\frac{u_{0}}{L}C_{\sigma,\sigma}+\lambda\nabla^{2}C_{m,\sigma}\right] . \tag{5.19}$$

It is then straightforward to convert this equation to a scaling equation. First, we still have to leading order that $C_{\psi,\psi}$ is given by Eq. (4.1). Next, using the Gaussian nature of m, one finds

$$C_{m,\sigma}(12)=\psi_{0}\left[\frac{2S_{0}}{\pi}\right]^{1/2}f(x) , \tag{5.20}$$

where f is again defined by Eq. (4.3), and f and F are related by Eq. (4.2). Inserting these results into Eq. (5.19) leads to

$$\mu\mathbf{x}\cdot\nabla_{x}F=\nabla_{x}^{2}\left[u_{0}F+\frac{\lambda\psi_{0}}{L\psi_{0}^{2}}\left[\frac{2S_{0}}{\pi}\right]^{1/2}\nabla_{x}^{2}f\right] , \tag{5.21}$$

where

$$\mu=\frac{L^{2}\dot{L}}{2D_{0}q_{0}^{2}} \tag{5.22}$$

and we make the initial choice $L^2=\pi S_0$. If we change characteristic lengths from L to $L_0=L/l$, then $\mathbf{x}\to\mathbf{x}/l$ and the scaling equation takes the form

$$\mu\mathbf{x}\cdot\nabla_{x}F=\nabla_{x}^{2}\left[l^{2}u_{0}F+\frac{l^{4}\lambda\psi_{0}}{L\psi_{0}^{2}}\left[\frac{2S_{0}}{\pi}\right]^{1/2}\nabla_{x}^{2}f\right] . \tag{5.23}$$

If we choose l such that

$$1=\frac{l^{4}\lambda\psi_{0}}{\mu L\psi_{0}^{2}}\left[\frac{2S_{0}}{\pi}\right]^{1/2}=\frac{l^{4}\lambda\sqrt{2}}{\mu\pi\psi_{0}} \tag{5.24}$$

and define

$$\tilde{u}=\frac{u_{0}l^{2}}{\mu}=\frac{\pi\psi_{0}u_{0}}{\sqrt{2}l^{2}\lambda} , \tag{5.25}$$

then we have the fundamental scaling equation in this approximation

$$xF'=\nabla_{x}^{2}[\tilde{u}F+\nabla_{x}^{2}\sin(\pi F/2)] . \tag{5.26}$$

This is a nonlinear eigenvalue problem for F, with a unique solution under the boundary conditions Eq. (1.4) and $\lim_{x\to\infty}F=0$. We will see that $\tilde{u}$ is determined as part of the solution. The only parameter left to be specified externally is the dimension of the system, d, appearing in the spherically symmetric Laplacian.

B. Analytic results

1. *Short scaled distances*

As in the naive case, it is instructive to examine the small- and large-x behavior of F analytically. It is again useful to carry out a first integration and obtain

$$\tilde{u}F+\nabla^{2}\sin\frac{\pi}{2}F=\frac{1}{d-2}\left[\frac{dI_{d}(x)}{x^{d-2}}-2[I_{2}(x)-I_{2}(\infty)]\right] \tag{5.27}$$

with the integrals I_d are defined by Eq. (4.10). Inserting the short-distance form Eq. (1.4) into (5.27) gives, to $O(1)$ and $O(x)$, respectively,

$$\tilde{u}=\frac{\pi^2\alpha^2 d}{4}+\frac{2I_2(\infty)}{d-2}\ , \tag{5.28}$$

$$\tilde{u}=-3\pi^2(d+1)\alpha\beta_2/4\ . \tag{5.29}$$

The interpretation of the short-distance parameters is now different from the NCOP and naive cases where α is given by Eq. (4.7). In this case, we find that α and β_2 are undetermined, and the two eigenvalues to be found in this case during the numerical solution of Eq. (5.27), can be taken to be α and β_2. It will turn out that $\beta_2\neq 0$, so that again, as in the naive theory, F does not satisfy the Tomita sum rule. Notice, using Eq. (5.25) that the ratio u_0/λ is determined once α, β_2, and l^2 are determined.

2. Long scaled distances

At large scaled distances, F decays to zero and Eq. (5.26) reduces to the same linear equation for F as for the naive case except with $\mu_0=2/\pi$. Therefore, F is again given by Eq. (4.8), but with this specific choice for μ_0.

3. Spatial moments

The small Q behavior of $\tilde{F}(Q)$ can be related to the moments of $F(x)$, defined by Eq. (4.12), as in the naive case. Multiplying Eq. (5.26) by x^p and integrating, we find $W_0=W_2=0$ and

$$W_4=-\frac{8d(d+2)}{(d+4)}W_f\ , \tag{5.30}$$

where

$$W_f=\int d^dx f(x)\ . \tag{5.31}$$

We thus have $\tilde{F}=\mathcal{Q}_4Q^4$ to lowest order in Q as desired, with

$$\mathcal{Q}_4=-\frac{1}{(d+4)}W_f\ . \tag{5.32}$$

Notice, however, because of the minus sign, that there is again a problem. Either $\mathcal{Q}_4$ or W_f must be negative, while mathematically, from their definitions, both must be positive. We will see below that $\tilde{F}$ is positive definite, and thus

$$W_f=\lim_{q\to 0}\langle|m_q(t)|^2\rangle/S_0<0\ . \tag{5.33}$$

As pointed out by Yeung, Oono, and Shinozaki [5], this is a short coming of the assumption that $m(\mathbf{R},t)$ is a Gaussian variable.

C. Numerical results

The numerical solution of the scaling equation Eq. (5.27) involves a nonlinear eigenvalue problem where α and β_2 must be chosen to satisfy the boundary conditions at small and large x. We find $\alpha=1.1262$, $\beta_2=-0.2650$ in $d=2$ and $\alpha=0.965\,622$, $\beta_2=-0.252\,672$ in $d=3$. Figures 1 and 2 compare our $d=3$ correlation function and structure factor, respectively, with recent numerical results of Shinozaki and Oono [12]. We have normalized their data so that the first zero of F coincides with ours.

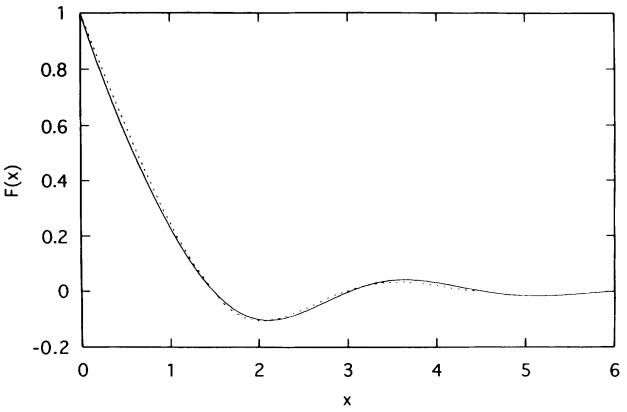

FIG. 1. Comparison of the theoretical scaling function $F(x)$ in the GDA with the numerical result (dashed line) from Ref. [12].

We see that there is good agreement for $F(x)$ but only fair agreement for $\tilde{F}(Q)$. The width of $\tilde{F}(Q)$ given by the theory is too narrow compared to the numerical result. It is worthwhile noting that the $\tilde{F}(Q)$ obtained in the naive theory [24] is too broad compared to the numerical result. This makes sense since the naive theory has $\tilde{F}\approx Q^2$ for small Q and β_2 is much smaller than in the GDA. In some sense, the theory has over corrected and the value of $\mathcal{Q}_4$ is too small. The auxiliary quantity $f(x)$ and its Fourier transform $\tilde{f}(Q)$ are shown in Figs. 3 and 4. Note the negative portion of $\tilde{f}(Q)$ for small Q. Reading off the numerically determined value to be $W_f=-0.23,\ldots,$ we obtain $\mathcal{Q}_4=0.033\ldots$.

D. Very short-distance behavior

The steps leading from Eq. (5.1) to the scaling result Eq. (5.26) relies on the assumption that one is looking at distances $R\gg\xi$, where, for example,

$$C_{\sigma_2,\sigma}(\mathbf{R},t)\approx O(L^{-2})\ . \tag{5.34}$$

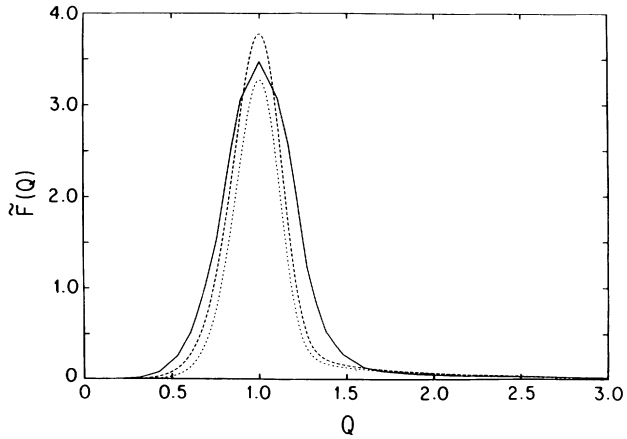

FIG. 2. Comparison of the theoretical scaling functions $\tilde{F}(Q)$ in the GDA (long-dashed curve) and PGA (short-dashed curve) with the numerical result from Ref. [12]. All curves have been normalized to have the same peak position.

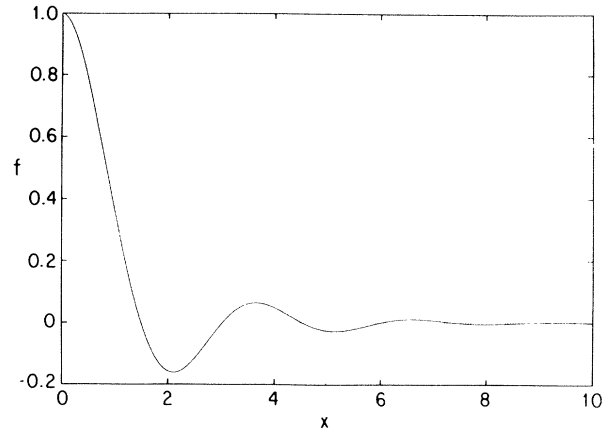

FIG. 3. Autocorrelation function f for the auxiliary field m for the GDA in three dimensions.

In contrast, for separations $R \approx \xi$

$$C_{\sigma_2,\sigma}(\mathbf{R},t) \approx O(L^{-1}) \tag{5.35}$$

and the evaluation of Eq. (5.1) is more complicated. As will be shown below, the matching of the short- and long-distance behavior results in an additional constraint on the parameters u_0 and λ.

An important aspect of this calculation is that it gives, self-consistently, the quantities $S_0^{(2s)}$. In the NCOP case, as $L \to \infty, S_0^{(2)} = \frac{1}{2}$, but in the COP case we obtain more involved results. It is also important to recognize that for the scaling limit associated with the LSW growth law to be consistent, one must have the self-consistent result $S_0^{(4)}$ vanish at least as fast as $O(L^{-1})$. In our analysis, here, we assume that $S_0^{(4)} \approx O(L^{-2})$ and defer discussion of this quantity for now.

The short-distance evaluation of Eq. (5.1) has the leading contribution of $O(L^{-1})$ which has the form

$$\nabla_R^2 \Sigma(\mathbf{R},t) = 0 \ . \tag{5.36}$$

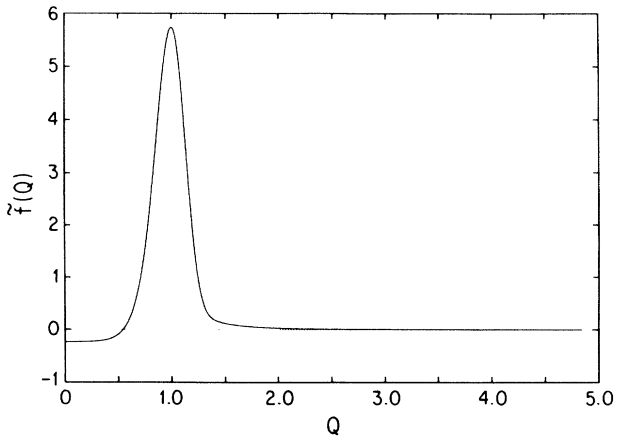

FIG. 4. Fourier transform of the autocorrelation function for the auxiliary field m for the GDA in three dimensions.

In evaluating $\Sigma(\mathbf{R},t)$, given by Eq. (5.3), one begins with the expansion

$$C_0(\mathbf{R},t) = S_0 - \frac{R^2}{2d} S_0^{(2)} + \cdots \ . \tag{5.37}$$

Terms higher than $W^{(2)}$ do not contribute at this lowest order of L^{-1} and one then has that $\nabla^2 \Sigma(\mathbf{R},t)|_{\mathbf{R}=0}$, at $O(L^{-1})$, is given by

$$\frac{1}{\sqrt{2}} S_0^{(2)} \left[\int_{-\infty}^{\infty} dx \, \sigma_2^2(x) \right] \left[\frac{1}{2} - S_0^{(2)} \left[1 + \frac{2}{d} \right] \right] = 0 \ , \tag{5.38}$$

which reduces to

$$S_0^{(2)} = \frac{d}{2(2+d)} \ . \tag{5.39}$$

Note, as for the NCOP case, $S_0^{(2)}$ is independent of the details of the potential.

The other limit of interest at $O(L^{-1})$ is where $\xi \ll R \ll L$. This regime is discussed in detail in the Appendix. In this case, one obtains a matching condition between the short-distance behavior and the scaling behavior. This condition, with $\tilde{\alpha} = \alpha l$, is given by

$$-1 + \frac{\pi}{2} \tilde{\alpha}^2 (d-1) - \lambda^2 y^2 \Delta_1 - \lambda y \Delta \bar{V}^{(2)} / \psi_0 = 0 \ , \tag{5.40}$$

where $\Delta \bar{V}^{(2)}$ is given in the Appendix by Eq. (7.11), Δ_1 is defined by Eq. (5.15), and

$$y = S_0^{(2)} - \frac{d\pi}{4} \tilde{\alpha}^2 \ . \tag{5.41}$$

In the case where $\lambda = 0$, we go back to the old result for $\tilde{\alpha}$ given by Eq. (4.7). Note that λ does depend on the details of the potential through Δ_1, ψ_0, etc.

E. Parameters

At this stage all of the various parameters can be determined in terms of the single parameter l, and properties of the potential. Since y is a function of d, α (which is determined as a solution of the eigenvalue problem) and l, λ can be determined as a function of l, d and properties of the potential using Eq. (5.40). These values of λ are then inserted into

$$-\frac{3\pi^2}{4}(d+1)\alpha\beta_2 = \frac{\pi\psi_0}{\sqrt{2}\lambda l^2} u_0 \tag{5.42}$$

to determine u_0 in terms of l, d, and properties of the potential. Finally, the amplitude in the growth law is determined by

$$\mu = \frac{\sqrt{2}\lambda l^4}{\pi\psi_0} \ . \tag{5.43}$$

In the case of the ψ^4 potential, where $\Delta_1 = 6$, $q_0^2 = 2$, and $\Delta \bar{V}^{(2)} = -6$, the solution of Eq. (5.40) is given in three dimensions by

$$\lambda=\frac{5\left[1\pm\left[\frac{1+2\pi(\alpha l)^2}{3}\right]^{1/2}\right]}{3\left[1-\frac{5\pi}{2}(\alpha l)^2\right]}, \tag{5.44}$$

and

$$u_0=-3\sqrt{2}\pi\alpha\beta_2\lambda l^2 . \tag{5.45}$$

The situation here where l is undetermined is unlike the NCOP and naive cases where there are no undetermined parameters—the scaling function and the characteristic growth law are fixed. In the case discussed here, the overall amplitude of the growth law $L(t)$ is not fixed by the scaling equation. There are a number of ways of obtaining an additional equation for l. The most practical choice for the GDA is to look at the results of fixing the scale used for $F(x)$. Suppose the position of the first zero in the scaling function is determined, using some other method, to be given by $R_0(t)=\bar{R}(2D_0q_0^2t)^{1/3}$. In our theory here, we have that

$$R_0(t)=rL_0(t)=rL(t)/l , \tag{5.46}$$

where we find explicitly from our numerical solution in three dimensions that $r=1.49,\ldots$. Furthermore, using Eqs. (5.22) and (5.24), we have that

$$L(t)=\bar{L}(2D_0q_0^2t)^{1/3} , \tag{5.47}$$

where

$$\bar{L}^3=\frac{3l^4\lambda\sqrt{2}}{\pi\psi_0} . \tag{5.48}$$

Equating the two expressions for $R_0(t)$ gives

$$(\bar{R}/r)^3=\frac{3\sqrt{2}\lambda l}{\pi\psi_0} . \tag{5.49}$$

For a given $\bar{R}$, this equation, together with Eq. (5.44), determines λ and l and allows a direct comparison with numerical studies of the same problem. Note that these statements are dependent on the form of the potential.

VI. POST-GAUSSIAN APPROXIMATION

A. Equations of motion

In this section, the theory is extended to include the first nontrivial post-Gaussian approximation where averages are over $P[m]$ given by Eq. (3.25) with all $A_n=0$ except for $n=0$ and 2. We call this the post-Gaussian approximation (PGA). For simplicity here we restrict the analysis to the case of equal times $t=t_1=t_2$. The scaling properties can be expressed in terms of the two quantities $f(x)$ and

$$g(x)=\frac{A_2(\mathbf{R}_1-\mathbf{R}_2,t)}{S_o(t)} . \tag{6.1}$$

In this case, $g(x)$ is a measure of the non-Gaussian corrections. One has by construction $f(0)=1$. In this analysis, one sees that in evaluating two-point averages in the scaling regime that $g(0)$ is typically multiplied by factors of γ [defined by Eq. (4.4)]. Since as R goes to 0, f goes to 1 and γ blows up, for consistency, we must choose $g(0)=A_2(11)=0$. Since this result simplifies the subsequent analysis considerably we enforce this condition at the beginning.

The technical results necessary to carry out averages for the $n=2$ model are outlined in the Appendix of Ref. [3]. One finds, for example, that the order parameter scaling function is related to f and g by

$$F(x)=\frac{2}{\pi}[\sin^{-1}f+2\gamma g] , \tag{6.2}$$

where γ is defined by Eq. (4.4).

It was suggested above and in Ref. [3] that for a probability distribution $P[m]$ characterized by coefficients $[C_0, A_2, A_4, \ldots, A_n]$ one can impose $n+1$ conditions of the form

$$\langle\tilde{B}(1)\sigma(2)\sigma(3)\cdots\sigma(n+1)\rangle=0 . \tag{6.3}$$

In Ref. [3] for the NCOP problem, it was shown that for the case where $P[m]$ is characterized by $[C_0, A_2]$ one can enforce essentially all one and two-point averages of the form

$$\Omega_n(1)=\langle B(1)\sigma^{2n+1}(1)\rangle=0 , \tag{6.4}$$

$$\Omega^O_{n,l}(12)=\langle B(1)\sigma^{2n}(1)\sigma^{2l+1}(2)\rangle=0 , \tag{6.5}$$

$$\Omega^E_{n,l}(12)=\langle B(1)\sigma^{2n+1}(1)\sigma^{2l}(2)\rangle=0 , \tag{6.6}$$

for integers n and l and the superscripts O and E stand for *odd* and *even* sectors. In the case of a COP one cannot satisfy all of the $\Omega^O_{n,l}$ for all n and l. Indeed we must be less ambitious and require [25]

$$\Omega_0(1)=\langle\tilde{B}(1)\sigma(1)\rangle=0 , \tag{6.7}$$

$$\Omega^O_{0,0}(12)=\langle\tilde{B}(1)\sigma(2)\rangle=0 , \tag{6.8}$$

and

$$\Omega^E_{0,0}(12)=\langle\tilde{B}(1)\sigma(1)\sigma^2(2)\rangle=0 . \tag{6.9}$$

B. Scaling regime

The evaluation of the condition $\Omega^O_{0,0}(12)=0$, in the scaling regime, leads to a result which looks very similar to the result obtained in the GDA. After carrying out the same rescalings and introducing the same parametrization, one obtains

$$xF'=\nabla_x^2[\tilde{u}F+\nabla_x^2(f+2g)] . \tag{6.10}$$

Notice that the only modification of the GDA result given by Eq. (5.26) is to replace f by $f+2g$ on the right-hand side.

The important new element in this case is the evaluation of the quantity $\Omega^E_{0,0}(12)=0$ in the scaling regime. This is a rather involved calculation. The main result needed to evaluate the various averages in the first nontrivial post-Gaussian approximation is, for a general

function G of m,

$$\langle G\rangle=\langle G\rangle_0+\int d1\,d2\,A_2(12)\left\langle\frac{\delta^2}{\delta m(1)\delta m(2)}G\right\rangle_0 , \tag{6.11}$$

where $\langle\ \rangle_0$ indicates a Gaussian average over m. We then obtain, after considerable algebra, that in the scaling regime the leading contribution is of $O(L^{-2})$ and is given by

$$\begin{aligned}[\Omega^E_{0,0}(12)-\Omega_0(1)\psi_0^2]/D_0=&M_{0,0}\left[-S_0^{(2)}-2A_2^{(2)}+2\left[1+\frac{2}{d}\right]S_0^{(2)}(S_0^{(2)}+4A_2^{(2)})\right]\\&+M_{0,2}\left\{(\nabla C_0)^2\left[-1+4\left[1+\frac{2}{d}\right]S_0^{(2)}+8\left[1+\frac{2}{d}\right]A_2^{(2)}\right]\right.\\&\left.+\nabla C_0\cdot\nabla A_2\left[-4+16\left[1+\frac{2}{d}\right]S_0^{(2)}(2)\right]\right\}\\&+M_{1,1}2S_0^{(2)}A_2^{(2)}\left[-1+2\left[1+\frac{2}{d}\right]S_0^{(2)}\right]+M_{1,3}A_2^{(2)}(\nabla C_0)^2\left[-2+8\left[1+\frac{2}{d}\right]S_0^{(2)}\right]\\&+2M_{0,4}(\nabla C_0)^2[(\nabla C_0)^2+8\nabla C_0\cdot\nabla A_2]+4M_{1,5}A_2^{(2)}(\nabla C_0)^4\end{aligned} \tag{6.12}$$

where the matrix elements $M_{n,l}$ are given by

$$M_{n,l}(12)=\langle\sigma_n^2(1)\Delta_l(2)\rangle_0 , \tag{6.13}$$

where

$$\Delta(1)=\sigma^2(1)-\psi_0^2 , \tag{6.14}$$

the integer subscripts n and l indicate derivatives and

$$A_2^{(2)}=\lim_{\mathbf{R}\to o}-\nabla_R^2 A_2(\mathbf{R},t) . \tag{6.15}$$

Since C_0 and A_2 decay to zero for large separations, one finds that the coefficient of $M_{0,0}$ must vanish. This gives the result

$$-S_0^{(2)}-2A_2^{(2)}+2\left[1+\frac{2}{d}\right]S_0^{(2)}(S_0^{(2)}+4A_2^{(2)})=0 . \tag{6.16}$$

This result also comes from the local calculation $\Omega_0(1)=0$ and with $A_2^{(2)}=0$ reduces to the result, Eq. (5.39), obtained in the GDA.

Returning to Eq. (6.12), one can evaluate the matrix elements $M_{n,l}$ in the scaling regime and find that each has the common factor

$$D_0\int_{-\infty}^{\infty}dx_1\sigma_2^2(x_1)\int_{-\infty}^{\infty}dx_2\Delta(x_2)\frac{\gamma^3(x)}{L^2} . \tag{6.17}$$

After introducing the notation

$$\omega=8\left[1+\frac{2}{d}\right]A_2^{(2)} , \tag{6.18}$$

$$\eta=\sqrt{1+\omega^2} , \tag{6.19}$$

scaling variables, and canceling the common factor, one obtains the basic equation determining the non-Gaussian correction function

$$g'=\frac{1}{4(2z+\omega-\eta)}\left[f'(z-\eta)+\frac{\pi fg}{f'}P\right] , \tag{6.20}$$

where

$$z=\frac{6\gamma^2(f')^2}{\pi} , \tag{6.21}$$

and

$$P=\tfrac{5}{3}z^2+(\omega-\eta)z-S_0^{(2)}(1+\omega-\eta) . \tag{6.22}$$

Finally, in coupling this equation with the equation determining F, we must remember to rescale the scaled distance $x\to x/l$. This involves introducing

$$\tilde{z}=l^2z \tag{6.23}$$

to obtain

$$g'=\frac{1}{4(2\tilde{z}+\omega-\eta)}\left[f'(\tilde{z}-\eta)+\frac{\pi fg}{l^2f'}\tilde{P}\right] , \tag{6.24}$$

$$\tilde{P}=\tfrac{5}{3}\tilde{z}^2+(\omega-\eta)\tilde{z}-S_0^{(2)}(1+\omega-\eta) . \tag{6.25}$$

The nature of the problem is now clear. We have a coupled set of equations, (6.24) and (6.10) for f and g, respectively, which we expect to form an eigenvalue problem. Again we will have eigenvalues α and β_2, just as for the Gaussian case, but now with the additional variables $A_2^{(2)}$ and l. The inclusion of $A_2^{(2)}$ as an eigenvalue is familiar from the NCOP case. The introduction of the parameter l, which does not enter the GDA, is introduced here only through the equation for g. One proceeds as in previous cases by analyzing the short- and long-distance behaviors and then numerically searching for the associated nonlinear eigenvalue problem which connects these physically acceptable behaviors.

C. Analytical results

1. Short-distance behavior

In looking at the short scaled distance behavior, we have the expansions

$$f=1-\alpha_0 x^2-\beta_0 x^3+\cdots \tag{6.26}$$

and

$$g=-g_0 x^2-g_1 x^3+\cdots . \tag{6.27}$$

The expansion coefficients for F given by Eq. (1.4) are related to these coefficients by

$$\alpha=\frac{2}{\pi}\sqrt{2\alpha_0}\left[1+\frac{g_0}{\alpha_0}\right], \tag{6.28}$$

$$\beta_2=\frac{2g_1+\beta_0(1-g_0/\alpha_0)}{2(\alpha_0+g_0)} . \tag{6.29}$$

Using these results in the equation for F leads to the generalizations of Eqs. (5.28) and (5.29):

$$\tilde{u}-2d(\alpha_0+2g_0)=\frac{2I_2(\infty)}{(d-2)} \tag{6.30}$$

and

$$-\alpha\tilde{u}-3(d+1)(\beta_0+2g_1)=0 . \tag{6.31}$$

The equation for g, Eq. (6.24), then gives the results

$$g_0=\frac{\alpha_0(z_0-\eta)}{4(2z_0+\omega-\eta)+3z_1/z_0} , \tag{6.32}$$

$$g_1=\frac{\beta_0\{7z_0-3\eta+(g_0/\alpha_0)[9z_1/z_0-32z_0-12(10z_0/3+\omega-\eta)]\}}{12(2z_0+\omega-\eta)+6z_1/z_0} , \tag{6.33}$$

where

$$z_0=\frac{12I^2\alpha_0}{\pi} , \tag{6.34}$$

and

$$z_1=\tfrac{5}{3}z_0^2+(\omega-\eta)z_0-S_0^{(2)}(1+\omega-\eta) . \tag{6.35}$$

2. Long-distance behavior

We find for large x that f and g will decay to zero and we find that Eq. (6.10) reduces to the same linear equation satisfied by F in the Gaussian case. Thus, asymptotically F shows the same damped exponential behavior as in the Gaussian case as given by Eq. (4.6). If one looks individually at f and g, one finds something very interesting. f and g individually decay less rapidly than F. f and g decay as $\exp-\kappa x$ while the sum $F=f+2g$ decays exponentially but with an exponent proportional to $x^{4/3}$. It is not difficult to determine the decay constant κ governing f and g. We assume

$$f=f_\infty\exp(-\kappa x) , \tag{6.36}$$

$$g=g_\infty\exp(-\kappa x) , \tag{6.37}$$

where

$$f_\infty+2g_\infty=0 \tag{6.38}$$

and find, after inserting these forms into the linearized version of Eq. (6.24),

$$\kappa^2=\frac{\pi S_0^{(2)}(1+\omega-\eta)}{2(3\eta-2\omega)I^2} . \tag{6.39}$$

The key point here is that the large x form for f does not oscillate with distance. This is qualitatively different from the Gaussian case and the first indication of the significant difference in the form of f in this case.

3. Spatial moments

Turning to the moments which govern the small Q behavior of $\tilde{F}(Q)$ and $\tilde{f}(Q)$, we find the easy generalization of Eq. (5.32) for the coefficient of the Q^4 term in the small Q expansion of the structure factor $\tilde{F}(Q)$ to be given by

$$\mathcal{Q}_4=-\frac{1}{(d+4)}\int d^3x[f(x)+2g(x)] . \tag{6.40}$$

Since we shall find in this case that $f(x)$ is positive for all x we see that it is the sum $f+2g$ whose integral must be negative, if $\mathcal{Q}_4$ is to be positive. This is discussed in more detail below.

D. Conservation laws

In the previous work on this problem, it has not been difficult to construct the theory such that the order parameter autocorrelation function satisfy the conservation law

$$\frac{d}{dt}\int d^dR\,C_{\psi,\psi}(\mathbf{R},t)=0 . \tag{6.41}$$

This was basically guaranteed in the current theory by satisfying the equation of motion given by $\Omega^O_{0,0}(12)=0$. Consider the more general correlation function

$$C_{\psi,G}(12)=\langle\psi(1)G(2)\rangle , \tag{6.42}$$

where G is not conserved. In terms of Fourier transforms and apart from uninteresting terms which depend on the initial conditions, one expects

$$C_{\psi,G}(\mathbf{q},t_1,t_2)=\langle\psi(\mathbf{q},t_1)G(-\mathbf{q},t_2)\rangle \tag{6.43}$$

$$\approx q^2 \tag{6.44}$$

for small q. Is the theory developed here compatible with this general result? Let us carry out the calculation of $C_{\psi,G}$ in the scaling regime. To leading order in the scaling regime where

$$\psi=\tilde{\psi}=\sigma\left[1-\frac{u_0}{L}\right]-\lambda\nabla^2 m\ , \tag{6.45}$$

it is clear that the condition that $C_{\psi,G}$ is conserved can be replaced by the condition that

$$C_{\sigma,G}(\mathbf{q},t_1,t_2)\approx q^2 \tag{6.46}$$

for small q. We therefore need to calculate $C_{\sigma,G}$ in the scaling limit using our lowest order post-Gaussian approximation. We have quite generally

$$C_{\sigma,G}(12)=C^{(0)}_{\sigma,G}(12)+2A_2(12)C^{(0)}_{\sigma_1,G_1}(12)\ ,$$

$$=C^{(0)}_{\sigma,G}(12)+2A_2(12)\frac{\partial}{\partial C_0(12)}C^{(0)}_{\sigma,G}(12)\ , \tag{6.47}$$

where $C^{(0)}_{\sigma,G}$ indicates the correlation function evaluated in the Gaussian approximation. The second step in Eq. (6.47) follows from a general theorem proven in Ref. [2] regarding the derivatives of correlation functions with respect to C_0. It is then not difficult to show, in the scaling regime, that

$$C^{(0)}_{\sigma,G}(12)=-\frac{2\psi_0}{L^2}\left[\int_{-\infty}^{\infty}dx_1 x_1 G(x_1)\right]f(12)\gamma(12)\ , \tag{6.48}$$

where we assume that G is a local functional of σ and vanishes as $|m|\to\infty$. This last restriction is not severe for the following reason: Consider a general $G=G(\sigma)$ which is odd in σ since $C_{\sigma,G}$ vanishes by symmetry otherwise. Then, if as $m\to\pm\infty$, $\sigma\to\pm\psi_0$, one can write

$$G=G_0\sigma+\Delta G\ , \tag{6.49}$$

where $\Delta G\to 0$ as $|m|\to\infty$. Then one can write

$$C_{\sigma,G}(12)=G_0 C_{\sigma,\sigma}(12)+C_{\sigma,\Delta G}(12) \tag{6.50}$$

and we can restrict further arguments to $C_{\sigma,\Delta G}(12)$ as indicated above since $C_{\sigma,\sigma}(q)\approx O(q^4)$ for small q. Inserting Eq. (6.48) into Eq. (6.47) gives

$$C_{\sigma,G}(12)=-\frac{2\psi_0}{L^2}\left[\int_{-\infty}^{\infty}dx_1 x_1 G(x_1)\right]\times\left[f(12)\gamma(12)+2A_2(12)\frac{\partial}{\partial C_0(12)}f(12)\gamma(12)\right]\ . \tag{6.51}$$

It is easy to see that

$$\frac{\partial(f\gamma)}{\partial C_0}=\frac{\gamma^3}{S_0}\ , \tag{6.52}$$

and we have the final result

$$C_{\sigma,G}(12)=-\frac{2\psi_0}{L^2}\left[\int_{-\infty}^{\infty}dx_1 x_1 G(x_1)\right]\gamma(12)\times[f(12)+2g(12)\gamma^2(12)]\ . \tag{6.53}$$

Therefore, for any $G(\sigma)$ in this class, the conservation law is satisfied if the integral of $C_{\sigma,G}$ over all (scaled) distances vanishes:

$$\int d^d x\gamma(x)[f(x)+2g(x)\gamma^2(x)]=0\ . \tag{6.54}$$

Notice that this result does not depend on the particular form of G.

In the Gaussian approximation this constraint reduces to the requirement

$$\int d^d x\gamma(x)f(x)=W_{\tan}=0\ . \tag{6.55}$$

We found earlier, however, that $W_{\tan}>0$, so the Gaussian approximation is incompatible with this manifestation of the conservation law. In the post-Gaussian approximation we find that it is possible to satisfy this constraint.

E. Numerical results ($d=3$)

The first step in solving the coupled pair of equations, Eqs. (6.10) and (6.24) is to carry out the same first integration as led from Eq. (5.26) to Eq. (5.27) on Eq. (6.10). We then have a second-order differential equation for $f+2g$ and a first-order differential equation for g. This second-order equation for $f+2g$ can be converted into a second-order equation for f by taking another derivative of g' which is used in $f''+2g''$ to eliminate g''.

There are four basic input parameters in this problem: α_0, β_0, l^2, and $A_2^{(2)}$. This is a large parameter space to search for solutions to this rather complicated set of equations. In looking at the role of the four parameters involved in the analysis we find that they divide into two sets. The set of parameters $A_2^{(2)}$ and l^2 did not enter into the Gaussian case. The other set is α_0 and β_0, which are equivalent to α and β_2 in the Gaussian case ($\alpha_0=\pi^2\alpha^2/8$, $\beta_0=2\beta_2/\alpha_0$). We find that this last set of parameters take on approximately the same values in the post-Gaussian case as in the Gaussian case. The numerical work has thus far been limited to three dimensions. Looking in this region and for small values of $A_2^{(2)}$ ($0.0001<A_2^{(2)}<0.0024$), we have found at least one branch of physically acceptable solutions. We have not looked for smaller values of $A_2^{(2)}$ and have not been able to find physically acceptable solutions for $A_2^{(2)}>0.0032$. By a physically acceptable solution, we mean one which satisfies the conservation law

$$\int d^d xF(x)=0\ . \tag{6.56}$$

One obtains these physical solutions only for a band of

small values of l^2 for each small value of $A_2^{(2)}$. Thus, for example, for $A_2^{(2)}=0.0016$, we find physically acceptable solutions for the approximate range of values $0.0340<l^2<0.0530$. A very interesting point is that, for each physically acceptable value of $A_2^{(2)}$, one can find a value for l^2 for which one can satisfy the conservation law constraint given by Eq. (6.54). This line of solutions is shown in Fig. 5. For larger values of $A_2^{(2)}$, because of instabilities associated with g becoming positive, we have not been able to find physically acceptable solutions. On the other hand, for these sets of parameters, the coefficient of the Q^4 term in $\tilde{F}(Q)$ is slightly negative. If one abandons satisfying the higher-order conservation law, then one can find values of l^2 for which the coefficient of Q^4 in the structure factor is very small but positive. A key observation is that the scaling function itself, shown in Fig. 6, and the structure factor, shown in Fig. 3, except for the small Q behavior is rather unaffected by the particular choices of $A_2^{(2)}$ and l^2 within the physically acceptable band of solutions. The results presented here are for $A_2^{(2)}=0.000\,159$, $l^2=0.003\,75$, $\alpha_0=0.9687,\ldots,$ $\beta_0=-0.5012,\ldots$. These values correspond to $\alpha=1.0120\ldots$ and $\beta_2=-0.2619$. In this case, we have that the coefficient of the Q^4 term is positive but very small.

By far the most important qualitative change in the analysis between the Gaussian and post-Gaussian cases is that the quantity f, which is oscillatory in the Gaussian case (see Fig. 3), becomes positive in the post-Gaussian case (see Fig. 7). Thus the qualitative feature that the Fourier transform of f goes negative for small wave numbers is clearly removed and the theory is put on much firmer ground in the COP case. Qualitatively, what happens in this case is that f and $-2g$, which are both positive, subtract to give the oscillatory behavior of F. Note, as in the NCOP case, the quantity g, shown in Fig. 7, while not large, is quantitatively significant even though $A_2^{(2)}$ is very small. A full probe of possible solutions of the coupled set of equations is numerically time consuming but straightforward.

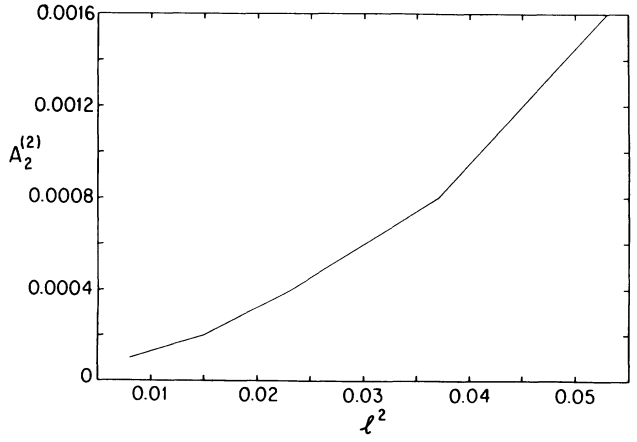

FIG. 5. Line of solutions in the PGA which satisfy the conservation law Eq. (6.54) in three dimensions.

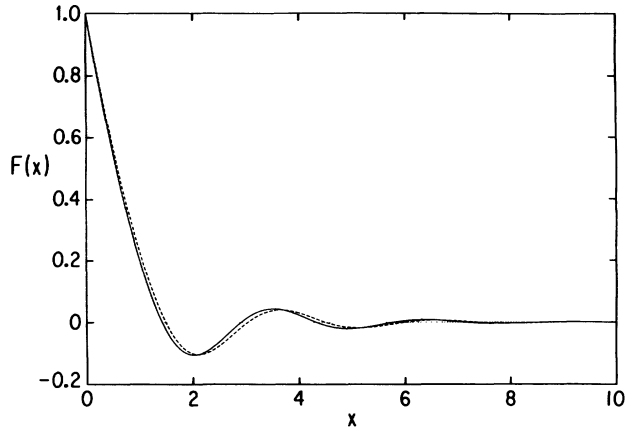

FIG. 6. Comparison of the theoretical scaling function $F(x)$ in the PGA with the GDA result (dashed line). Notice that in this case, we did not fix the lengths such that the two curves share the same first zero as was arranged in Fig. 1.

In Figs. 1, 2, and 6 we show the comparison among the $F(x)$ and $\tilde{F}(Q)$ in the GDA and PGA and with the numerical work of Ref. [12]. We see that in coordinate space the comparison is good. The agreement for the structure factor is not as good. While the fit to the Porod tail and the peak height is pretty good for both the GDA and PGA, the width of the theoretical structure factors is much narrower than for the numerical results. This can be partially attributed to the very small coefficients of Q^4 found in the theory. This point requires further study.

F. Short-distance matching

The generalization of the result Eq. (5.40) to the PGA is given by

$$\frac{4}{\pi}\alpha_0 l^2(d-1)\frac{1+2g_0/\alpha_0}{1-g_0/\alpha_0}-1-\lambda Y\Delta V^{(2)}/\psi_0-(\lambda Y)^2\Delta_1 =0\ , \quad (6.57)$$

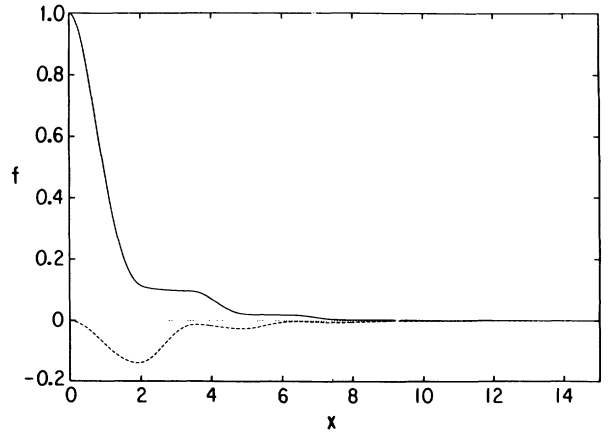

FIG. 7. Autocorrelation function f for the auxiliary field m for the PGA in three dimensions. Also shown (dashed line) is the quantity g.

where

$$Y=S_0^{(2)}+A_2^{(2)}-\frac{2d}{\pi}(\alpha_0+2g_0)l^2 . \tag{6.58}$$

VII. CONCLUSIONS

A more general approach to the theory of growth kinetics, which goes beyond the limitations of the Gaussian approximation for the appropriate auxiliary field, has been presented for the COP case. The theory is developed in terms of a rather general probability distribution characterized by a set of functions $[C_0, A_2, A_4, \ldots,]$. It is shown that if one truncates this set at low-order averages of the original equation of motion can be used to determine, for example, C_0 and A_2. It is very encouraging that the simple set $[C_0, A_2]$ leads to a theory which is qualitatively improved over the Gaussian case.

It is clear from this and previous work that the COP case is considerably more constrained than the NCOP case and the long-distance, small wave-number properties are very delicate. However, we believe that in this work we have been able to gain some insight and control over the type of theory needed to handle this part of the problem. Indeed, from the point of view of the scaling function, for all but the largest scaled distances the theory appears to be very good. At the longest distances, we see that there are a number of competing constraints:

$$\int d^dx F(x)=0 , \tag{7.1}$$

$$\int d^dx x^2 F(x)=0 , \tag{7.2}$$

$$\int d^dx x^4 F(x)=-\frac{8d(d+2)}{d+4}\int d^dx\,[f(x)+2g(x)]>0 , \tag{7.3}$$

$$\int d^dx \gamma(x)[f(x)+2g(x)\gamma^2(x)]=0 , \tag{7.4}$$

and

$$\int d^dx f(x)>0 . \tag{7.5}$$

In the naive theory, where $g=0$, (7.1) and (7.2) are the only constraints satisfied. In the GDA, where again $g=0$, (7.1), (7.2), and (7.3) are satisfied but (7.4) and (7.5) cannot be satisfied. In the PGA one can satisfy (7.1), (7.2), and (7.5) easily, but one cannot apparently, simultaneously satisfy (7.3) and (7.4). Thus, one is gaining progressive control over these properties and it should be clear that it is likely that by going to higher orders in the theory one will be able to satisfy the progressively more stringent constraints.

There remain several questions concerning the PGA. One question concerns a more exhaustive analysis of the numerical solutions as a function of $A_2^{(2)}$ and l^2. It is not yet completely clear how the parameter l^2 should be interpreted. At this stage the identification of l^2 as in the treatment of the GDA seems operative. This does not, however, appear to be final since it would seem to imply that l^2 and, therefore, $F(x)$ are nonuniversal. It seems more likely that in a higher-order approximation, where conditions (c) and (d) above can be simultaneously satisfied, there will be a selection mechanism for l^2. For this reason it seems that one will have to go to the next order theory in order to obtain a good estimate for the coefficient of the Q^4 term in the structure factor.

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APPENDIX

In Sec. V D the short-distance behavior for the Gaussian model was discussed. As indicated there, the other limit of interest at $O(L^{-1})$ is where $\xi \ll R \ll L$, and where the short-distance and the scaling behavior must match. In this case, in evaluating Eq. (5.3), the basic results needed are

$$C_0(\mathbf{R},t)=S_0-\frac{\pi}{8}\tilde{\alpha}^2R^2(1+2\tilde{\beta}_2R/L+\cdots) , \tag{A1}$$

$$C_{0,0}(\mathbf{R},t)=\psi_0^2\left[1-\tilde{\alpha}\frac{R}{L}\left[1+\tilde{\beta}_2\frac{R}{L}+\cdots\right]\right] , \tag{A2}$$

where $\tilde{\alpha}=\alpha l$ and $\tilde{\beta}=\beta l$ are the short-distance coefficients before rescaling distances. One also needs the general result valid at $O(L^{-1})$, derived in Ref. [2], that for $R \ll L$, that

$$C_{AB}(\mathbf{R},t)=\int\frac{dx_1dx_2}{Lb\sqrt{2\pi}}\exp[-(x_1-x_2)^2/b^2]\times A(x_1)B(x_2) , \tag{A3}$$

where

$$b^2=4(S_0-C_0) , \tag{A4}$$

and, for large R,

$$b=b_\infty R+O(R^{-1})=\left[\frac{\pi}{2}\right]^{1/2}\tilde{\alpha}R \tag{A5}$$

for $R \gg \xi$. One can go further by recognizing that b_∞ must be related to the short-distance coefficient α associated with $F(x)$ and determined in the eigenvalue problem solved above. One easily finds

$$b_\infty=\left[\frac{\pi}{2}\right]^{1/2}\tilde{\alpha} \tag{A6}$$

for $R \gg \xi$. One also needs the recursion relation Eq. (5.12) to evaluate the quantities $W^{(l)}$. Only the first two matrix elements, $W^{(1)}$ and $W^{(2)}$, contribute in this limit from W. For large R and b, we obtain

$$\Sigma(\mathbf{R},t)=\frac{\bar{\Sigma}^{(\infty)}(\mathbf{R})}{L}+\frac{\bar{\Sigma}^{(b)}(\mathbf{R})}{bL}+\cdots , \tag{A7}$$

where

$$\bar{\Sigma}^{(\infty)}(\mathbf{R})=-u_0 q_0^2\psi_0+\lambda\gamma_0 q_0^2 d b_\infty^2 \tag{A8}$$

and

$$\bar{\Sigma}^{(b)}(\mathbf{R})=\frac{2\psi_0^2}{\sqrt{2\pi}}[-1+b_\infty^2(d-1)-\lambda^2 y^2\Delta_1 -\lambda y\Delta\bar{V}^{(2)}/\psi_0] , \tag{A9}$$

and we have defined

$$y=S_0^{(2)}-\frac{d}{2}b_\infty^2 , \tag{A10}$$

where

$$\Delta\tilde{V}^{(2)}=\int_{-\infty}^{\infty} dx\,\Delta V^{(2)}(\sigma(x)) \tag{A11}$$

and

$$\Delta V^{(2s)}(\sigma)=V^{(2s)}(\sigma)-q_{s-1}^2 . \tag{A12}$$

Since $\nabla^2\Sigma=0$, at this order, we have

$$-1+b_\infty^2(d-1)-\lambda^2 y^2\Delta_1-\lambda y\Delta\bar{V}^{(2)}/\psi_0=0 . \tag{A13}$$

In terms of $\tilde{\alpha}$, we have the result given by Eq. (5.40).

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[19] A. J. Bray and K. Humayun, Phys. Rev. E **48**, R1609 (1993).

[20] The ideas introduced in this section were developed in close collaboration with Eric Kramer.

[21] In Ref. [14], u was taken as an independent field unlike the case treated here.

[22] The sign convention is chosen because we expect u to decrease the ordered magnitude of ψ.

[23] Extending the theory to include, for example, the λ_3 term is easy, in principle, but in practice introduces higher-order gradients into the scaling equation of motion. It may be possible to satisfy the Tomita sum rule by including the λ_3 term in the expression for u_1.

[24] G. F. Mazenko (unpublished).

[25] This statement is a bit too restrictive. One can actually satisfy $\Omega_{0,l}^E(12)=0$ to leading order in L^{-1} for general l.