Post-Gaussian approximations in phase ordering kinetics

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Existing theories for the growth of order in unstable systems have successfully exploited the use of a Gaussian auxiliary field. The limitations imposed on such theories by assuming this field to be Gaussian have recently become clearer. In this paper it is shown how this Gaussian restriction can be removed in order to obtain improved approximations for the scaling properties of such systems. In particular it is shown how the improved theory can explain the recent numerical results of Blundell, Bray, and Sattler [Phys. Rev. E **48**, 2476 (1993)] which are in qualitative disagreement with Gaussian theories.

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I. INTRODUCTION

Essentially all of the current theories for the growth of order in unstable systems assume the existence of an underlying Gaussian auxiliary field. In the work of the author and co-workers [1–3], this variable $m(\mathbf{R},t)$ has the physical interpretation that its magnitude gives the distance from $\mathbf{R}$ to the nearest interface. In their theory for the case of a nonconserved order parameter (NCOP), Ohta, Jasnow, and Kawasaki [4] (OJK) introduce a Gaussian diffusion field u. These theories have had many successes, and the basic development has been pushed very far. The limitations of such theories has not been clear. When do they break down and how can one improve them? Direct comparisons of calculations with simulation results have shown that the "Gaussian" theories give good approximations for the order-parameter scaling function, and there has been difficulty in choosing among them. The OJK approach seems to give a better description for the order-parameter scaling function $F(x)$ for large scaled distances x, but the development due to the author gives a much better treatment for the nonequilibrium exponent λ associated with two-time correlation functions. Recent work by Blundell, Bray, and Sattler [5] (BBS) indicates that if one looks at higher-order correlation functions one finds a distinctive qualitative breakdown of the Gaussian descriptions for the auxiliary field. In this paper approximation methods are introduced which allow one to go beyond existing Gaussian approximations and obtain agreement with the test proposed by BBS.

In the case of a conserved order parameter (COP), the breakdown of Gaussian theories is signaled [6] by a crossover to negative values of the Fourier transform of the m-field autocorrelation function for small wave numbers. The development of post-Gaussian approximation for the COP case looks promising, but will be treated in subsequent work.

As mentioned above, Blundell, Bray, and Sattler [5] have recently proposed an "absolute test for theories of phase-ordering dynamics." They considered an ordering 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

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

versus the square of the order-parameter correlation function

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

has a qualitatively different behavior for small C_{ψ^2} than that predicted by existing Gaussian theories. Existing theories give

$$C_{\psi^2}=\frac{\pi^2}{8}[C_\psi/\psi_0^2]^2\ , \tag{3}$$

while the numerical work by BBS indicates that C_{ψ^2} goes to zero much faster than C_ψ^2 for small C_ψ. It seems clear that one must go beyond the Gaussian approximation to obtain this result.

We develop here a general theory 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.

II. PROBLEM STATEMENT

The theory discussed here has been applied to a variety of different ordering systems: Systems with a NCOP scalar order parameter are treated in Refs. [1,7–9], a NCOP $O(n)$-symmetric order parameter in Refs. [2,7,9–11], a NCOP q-state Potts model in Ref. [12], a COP scalar order parameter in Refs. [3,13], and a COP $O(n)$-symmetric order parameter in Ref. [14]. In all but the conserved scalar order-parameter case the application of the theory is a rather direct and simple application of the theory developed in Ref. [1]. Since many of the main points of the theory are apparent from the case of a scalar NCOP, the discussion here will be restricted to that case.

In the case of interest here, the dynamics of a scalar order parameter $\psi(\mathbf{R},t)$ are generated by a Langevin equation of the time-dependent Ginzburg-Landau (TDGL)

type:

$$\frac{\partial\psi}{\partial t}=-\Gamma[V'(\psi)-\nabla^2\psi]+\eta \ . \tag{4}$$

The noise η in Eq. (4), as usual, is assumed to be Gaussian with variance

$$\langle\eta(1)\eta(2)\rangle=2k_BT\Gamma\delta(12) \ , \tag{5}$$

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

$$\delta(12)=\delta(\mathbf{R}_1-\mathbf{R}_2)\delta(t_1-t_2) \ . \tag{6}$$

In Eq. (4), $V(\psi)$ is a degenerate, double-welled potential with minima at $\pm\psi_0$ and Γ is a kinetic coefficient. 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. In practice, one quenches from an initial state characterized by random (Gaussian) initial conditions with variance

$$\langle\psi_0(\mathbf{R})\psi_0(\mathbf{R}')\rangle=\epsilon_0\delta_{\mathbf{R},\mathbf{R}'} \ , \tag{7}$$

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,

$$\langle\psi(1)\rangle=0 \ . \tag{8}$$

It will be useful in the discussion below to rewrite the equation of motion Eq. (4) in the form

$$\Lambda(1)\psi(1)=-\Gamma V'(\psi(1))+\eta \ , \tag{9}$$

where

$$\Lambda(1)=\frac{\partial}{\partial t_1}+\Gamma(-\nabla_1^2) \ . \tag{10}$$

III. FORMAL DEVELOPMENT

A compact discussion of the method developed in Ref. [1] starts with the introduction of a translation of the order parameter of the form

$$\psi(1)=\sigma(1)+W(1)+u(1) \ , \tag{11}$$

where $u(1)$ is an independent fluctuating field and $\sigma(1)$ and $W(1)$ are to be determined. Next make the choice for $W(1)$ given by

$$W(1)=-\int d2G_u(12)B(2) \ , \tag{12}$$

where

$$B(1)=\Lambda(1)\sigma(1)+\Gamma V'(\sigma(1)) \tag{13}$$

and G_u is the Green's function

$$\Lambda_u(1)G_u(12)=\delta(12) \tag{14}$$

for the operator Λ_u:

$$\Lambda_u(1)=\Lambda(1)+\Gamma\Omega(1) \ , \tag{15}$$

where

$$\Omega(1)=\langle V''(\sigma(1))\rangle_\sigma \ . \tag{16}$$

In this last expression, the average is over an appropriate probability distribution governing the σ degrees of freedom to be discussed below. The original Langevin equation then takes the form

$$\Lambda_u(1)u(1)=\eta(1)-\Gamma U(1) \ , \tag{17}$$

where $U(1)$ is defined by

$$U(1)=V'(\sigma(1)+W(1)+u(1))-V'(\sigma(1))-\Omega(1)[W(1)+u(1)] \ . \tag{18}$$

The expectation is that $U(1)$ can be treated as a perturbation in the long-time limit. Equation (17) plus the supporting definitions are simply a redefinition of the original problem. There have been no approximations, and (17) is true for general choices for $\sigma(1)$.

The key points in the development, as first pointed out in Ref. [15], is that there should be a clear separation of the variables σ and u for long times, and if one is to get started on a quantitative theory, one should be able to neglect the *perturbation* U. As time evolves, the system orders and Ω becomes positive. This means that the propagator Λ_u, defined by Eq. (15), develops a *mass* and the u variable is rendered stable. This has the consequence that u decays exponentially to zero in the long-time limit and for quenches to $T=0$. For nonzero temperatures, for long times, the field u describes the fluctuations in an ordered domain.

If U is to be *small,* then one must require that W and B [which are linearly related by Eq. (12)] be small in the long-time limit. It is at this stage in the development where one has a choice. How are the degrees of freedom σ, which govern B, to be defined?

The key step, developed in Ref. [1], is the introduction of an auxiliary field m which is smoother than ψ, but whose zeros coincide with the interfaces of ψ. This field $m(\mathbf{R},t)$ has the physical interpretation that its magnitude gives the distance from $\mathbf{R}$ to the nearest interface. This physical picture can be realized by assuming that $\sigma(m)$ satisfies the equation for an equilibrium interface:

$$\tfrac{1}{2}\sigma_2(m)=V'(\sigma(m)) \ , \tag{19}$$

with m the associated coordinate. In Eq. (19) the factor $\frac{1}{2}$ is inserted for convenience, $\sigma_n(m)\equiv\partial^n\sigma(m)/\partial m^n$, and the boundary conditions are $\lim_{m\to\pm\infty}\sigma=\pm\psi_0$. It should be clear from the physics of the situation that at long times the fields m and u are essentially independent and should be viewed as fluctuating in separate function spaces. As such, as pointed out in some detail in Ref. [15], one must introduce a probability distribution $P[m]$ which governs the m fields. It is the average over $P[m]$ which appears in the definition of $\Omega(1)$.

Having transferred attention from σ to m, one is still left with the task of constructing B to be *small.* At the formal level, the simplest choice guaranteeing [11] that $B(1)$ be small is to choose

$$B(1)=\Lambda(1)\sigma(1)+\Gamma V'(\sigma(1))=0 . \quad (20)$$

This is equivalent to assuming that σ satisfy the original equation of motion with $\psi\rightarrow\sigma$ 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. In Ref. [1] a different approach was taken. Instead of taking $B(1)=0$, it was assumed that weighted averages of $B(1)$ are zero. Since $\langle B(1)\rangle_\sigma=0$ by symmetry, the simplest nonzero average is given by

$$\langle B(1)\sigma(2)\rangle_\sigma=0 . \quad (21)$$

Assuming that $P[m]$ is a Gaussian distribution, Eq. (21) is sufficient to determine the variance $\langle m(1)m(2)\rangle_\sigma$ and all other averages over m.

It was found in Ref. [1] 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 and $\Lambda(1)\sigma(1)$ and $V'(\sigma)$ approach zero in the long-time limit. Thus while $B(1)$ is not identically zero, it will be small. In the scaling regime, one estimates

$$B(1)\approx 1/t\approx 1/L^n , \quad (22)$$

where L is the growth law and n is the growth exponent.

The Gaussian approximation for $P[m]$, coupled with Eq. (21), leads to a very good zeroth-order approximation for the scaling function. Here we are concerned with the limitations of this theory. How does it break down and how could one improve it?

IV. POST-GAUSSIAN APPROXIMATIONS

How can one gain some control [16] over $P[m]$ in a near-Gaussian context? 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:

$$P[m]=e^{-K_0[m]}\sum_{n=0}^{\infty} A_n(1,2,\ldots,n)H_n(1,2,\ldots,n) , \quad (23)$$

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

$$H_n(1,2,\ldots,n)=(-1)^n e^{K_0[m]}\frac{\delta^n}{\delta m(1)\delta m(2)\cdots\delta m(n)}\times e^{-K_0[m]} , \quad (24)$$

where

$$K_0[m]=\frac{1}{2}\int d1\,d2\,m(1)C_0^{-1}(12)m(2) \quad (25)$$

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

$$\int d3 C_0^{-1}(13)C_0(32)=\delta(12) . \quad (26)$$

The set of functions $H_n(1,2,\ldots,n)$ form a complete orthogonal functional set in that any functional $d[m]$ can be expanded in the form

$$d[m]=\sum_{n=0}^{\infty}\int d1\,d2\cdots dn\,a_n(1,2,\ldots,n)\int d1'\,d2'\cdots dn'\,C_0(11')C_0(22')\cdots C_0(nn')H_n(1',2',\ldots,n') \quad (27)$$

and the expansion coefficients a_n are given by the averages

$$a_n(1,2,\ldots,n)=\frac{1}{n!}\langle d[m]H_n(1,2,\ldots,n)\rangle_0 , \quad (28)$$

where $\langle\ \rangle_0$ indicates an average over the Gaussian probability distribution

$$P_0[m]=\frac{e^{-K_0[m]}}{Z_0} , \quad (29)$$

and Z_0 is a constant chosen such that $P_0[m]$ is properly normalized $\langle 1\rangle_0=1$. Equation (28) follows from the orthogonality relations

$$\int d1''\,d2''\cdots dn''\,C_0(1'1'')C_0(2'2'')\cdots C_0(n'n'')\langle H_n(1,2,\ldots,n)H_{n'}(1',2',\ldots,n')\rangle_0 = \delta_{n,n'}I(1,2,\ldots,n;1',2',\ldots,n') , \quad (30)$$

where I is the product of δ functions which are symmetric under interchange of any two labels in the primed or unprimed set and conveniently defined by the functional derivatives

$$I(1,2,\ldots,n;1',2',\ldots,n')=\frac{\delta^n[m(1')m(2')\cdots m(n')]}{\delta m(1)\delta m(2)\cdots\delta m(n)} . \quad (31)$$

Carrying out averages over the general probability distribution $P[m]$ is rather convenient. It should be clear that essentially all averages of interest can be obtained from the generating functional

$$\mathcal{S}[D]=\left\langle \exp\left[\int d\bar{1}\, D(\bar{1})m(\bar{1})\right]\right\rangle$$
$$=\sum_{n=0}^{\infty}\int d1\, d2\cdots dn\; A_n(1,2,\ldots,n)\left\langle H_n(1,2,\ldots,n)\exp\left[\int d\bar{1}\, D(\bar{1})m(\bar{1})\right]\right\rangle_0 , \tag{32}$$

where $D(1)$ is an arbitrary function. The associated Gaussian average is straightforward to evaluate given the definition of the H_n with the final result

$$\mathcal{S}[D]=\sum_{n=0}^{\infty}\int d1\, d2\cdots dn\; A_n(1,2,\ldots,n)D(1)D(2)\cdots D(n)\exp\left[\int d\bar{1}\, d\bar{2}\frac{1}{2}D(\bar{1})D(\bar{2})C_0(\bar{1}\bar{2})\right] , \tag{33}$$

where

$$C_0(12)=\langle m(1)m(2)\rangle_0 . \tag{34}$$

Averages can be categorized by the number of distinct space-time points involved in the average. For example, all averages which depend on m at the same space-time point can be evaluated in terms of the quantity

$$\rho(x;1)=\langle\delta(x-m(1))\rangle$$
$$=\int\frac{dk}{2\pi}\langle e^{-ik[x-m(1)]}\rangle$$
$$=\int\frac{dk}{2\pi}e^{-ikx}\mathcal{S}[D(\bar{1})=ik\delta(\bar{1}1)] . \tag{35}$$

With this choice for D and the result (33), we easily obtain

$$\rho(x;1)=\sum_{n=0}^{\infty}A_n(1,1,\ldots,1)\int\frac{dk}{2\pi}e^{-ikx}(ik)^n e^{-k^2S_0(1)/2} , \tag{36}$$

where

$$S_0(1)=\langle m^2(1)\rangle_0 . \tag{37}$$

All of the coefficients A_n are evaluated at a single space-time point, and so one can define

$$A_n^{(0)}(1)\equiv A_n(1,1,\ldots,1) . \tag{38}$$

It is then easy to show that $\rho(x;1)$ can be written in the form

$$\rho(x;1)=\sum_{n=0}^{\infty}\frac{A_n^{(0)}(1)}{S_0^{n/2}}H_n(x/\sqrt{S_0})\frac{e^{-x^2/2S_0}}{\sqrt{2\pi S_0}} , \tag{39}$$

where the H_n are simply related to the usual set of Hermite polynomials. This result indicates that ρ is a function of $x/\sqrt{S_0}$ and that function can be expanded in terms of the complete set of Hermite polynomials. It also indicates that the natural set of expansion coefficients is given by

$$g_n^{(0)}(1)=\frac{A_n^{(0)}(1)}{S_0^{n/2}} \tag{40}$$

and that $A_n\sim L^n$.

Averages which depend on a single space-time point are given then by

$$\langle\phi[m(1)]\rangle=\int dx\;\phi[x]\rho(x;1) . \tag{41}$$

This can be expressed, after using the defining equation for the H_n and n integrations by parts, as

$$\langle\phi[m(1)]\rangle=\sum_{n=0}^{\infty}A_n^{(0)}(1)\langle\phi_n(1)\rangle_0 , \tag{42}$$

where we introduce the convenient notation

$$\phi_n[m(1)]\equiv\frac{d^n}{dm^n(1)}\phi[m(1)] . \tag{43}$$

Turning to the more interesting case of two-point averages, we easily find that

$$\rho(x_1,x_2;1,2)=\langle\delta(x_1-m(1))\delta(x_2-m(2))\rangle$$
$$=\int\frac{dk_1}{2\pi}\frac{dk_2}{2\pi}e^{-ik_1x_1-ik_2x_2}\mathcal{S}[D(\bar{1})=ik_1\delta(\bar{1}1)+ik_2\delta(\bar{1}2)]$$
$$=\int\frac{dk_1}{2\pi}\frac{dk_2}{2\pi}e^{-ik_1x_1}e^{-ik_2x_2}\sum_n\int d\bar{1}\, d\bar{2}\cdots d\bar{n}\,A_n(\bar{1},\bar{2},\ldots,\bar{n})[ik_1\delta(\bar{1}1)+ik_2\delta(\bar{1}2)][ik_1\delta(\bar{2}1)+ik_2\delta(\bar{2}2)]$$
$$\times\cdots[ik_1\delta(\bar{n}1)+ik_2\delta(\bar{n}2)]\exp\{-\tfrac{1}{2}[(k_1^2+k_2^2)S_0+2k_1k_2C_0(12)]\} . \tag{44}$$

This result, after doing the k_1 and k_2 integrations, can be put in the form

$$\rho(x_1,x_2;1,2)=\sum_{n=0}^{\infty}(-1)^n\sum_{s=0}^{n}\frac{n!}{s!(n-s)!}A_{n;s}(1,2)\frac{d^{n-s}}{dx_1^{n-s}}\frac{d^s}{dx_2^s}\rho_0(x_1x_2;12) , \tag{45}$$

where ρ_0 is the Gaussian result

$$\rho_0(x_1,x_2;12)=\frac{\gamma}{2\pi\bar{S}_0}\exp\left\{-\frac{\gamma^2}{2\bar{S}_0}[x_1^2+x_2^2-2x_1x_2f]\right\}, \tag{46}$$

where

$$f(12)=\frac{C_0(12)}{\bar{S}_0(12)}, \tag{47}$$

$$\bar{S}_0(12)=\sqrt{S_0(1)S_0(2)}, \tag{48}$$

and

$$\gamma(12)=[1-f^2(12)]^{-1/2}. \tag{49}$$

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 clear that general two-point averages can be written in the form

$$\begin{aligned}\langle\phi(1)\chi(2)\rangle&=\sum_{n=0}^{\infty}\sum_{s=0}^{n}\frac{n!}{s!(n-s)!}A_{n;s}(1,2)\langle\phi_{n-s}(1)\chi_s(2)\rangle_0\\&=\langle\phi(1)\chi(2)\rangle_0+A_2(11)\langle\phi_2(1)\chi(2)\rangle_0+2A_2(12)\langle\phi_1(1)\chi_1(2)\rangle_0\\&\quad+A_2(22)\langle\phi(1)\chi_2(2)\rangle_0+A_4(1111)\langle\phi_4(1)\chi(2)\rangle_0\\&\quad+4A_4(1112)\langle\phi_3(1)\chi_1(2)\rangle_0+6A_4(1122)\langle\phi_2(1)\chi_2(2)\rangle_0\\&\quad+4A_4(1222)\langle\phi_1(1)\chi_3(2)\rangle_0+A_4(2222)\langle\phi(1)\chi_4(2)\rangle_0+\cdots.\end{aligned} \tag{50}$$

Here we assume 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. If one includes $n=4$ terms, there are two additional independent functions $A_4(1112)$ and $A_4(1122)$.

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

$$\langle B(1)\sigma(2)\rangle_\sigma=0, \tag{51}$$

$$\langle B(1)\sigma(2)\sigma(3)\sigma(4)\rangle_\sigma=0, \tag{52}$$

etc., up to level n. In principle, as n increases, one might suppose that the theory enforces the condition that $B(1)$ be small more effectively. In the work here, we will look at the lowest-order versions of this theory. While this scheme might look unwieldy and arbitrary at first sight, we shall see below that it is practical and contains some elegant features. There are indications that the expansion sequence in n converges rather rapidly. We do not yet know why this may be the case.

In the next section, we review the theory obtained at the Gaussian level. This is followed in the next section by considering the case where we keep terms at level $n=2$.

V. GAUSSIAN THEORY

The case where $P[m]$ is Gaussian corresponds to $A_n=0$ for $n>0$. In this case we can only impose the single constraint

$$\langle B(1)\sigma(2)\rangle_0=0, \tag{53}$$

where $\langle\ \rangle_0$ indicates a Gaussian average. Equation (53) leads, in the scaling regime, to an equation for the variance $f(x)$. In evaluating the average given by (53) for the case of equal times $t_1=t_2=t$, we need the results

$$\langle\sigma(1)\sigma(2)\rangle_0=\psi_0^2F(x), \tag{54}$$

$$F(x)=\frac{2}{\pi}\sin^{-1}f(x), \tag{55}$$

and

$$\langle\sigma_2(1)\sigma(2)\rangle_0=-\frac{2\psi_0^2}{\pi S_0(1)}f\gamma \tag{56}$$

$$=-\frac{2\psi_0^2}{\pi S_0(1)}\tan\left[\frac{\pi}{2}F\right], \tag{57}$$

where $x=|\mathbf{R}_1-\mathbf{R}_2|/L$ and $L^2(t)\equiv\pi S_0(t)$. The equation of motion [Eq. (53)] in the case of equal times reduces to the scaling equation obtained in Ref. [1]:

$$-\mu_0\mathbf{x}\cdot\nabla F(x)=\tan\left[\frac{\pi}{2}F\right]+\nabla^2F, \tag{58}$$

where $2\Gamma\mu_0=L\dot{L}$. The solution of this equation is discussed in some detail in Refs. [1,17]. The key points involved in solving Eq. (58) follow from a study of its short- and long-distance solutions. For short-scaled distances, F is given by

$$F(x)=1-\alpha_0x(1+\beta_2x+\beta_3x^2+\cdots) \tag{59}$$

for small x, where

$$\alpha_0=\left[\frac{2}{\pi(d-1)}\right]^{1/2}, \tag{60}$$

$\beta_{\text{even}}=0$, and β_3 is given in [1]. For large x, where F is small, we can again solve Eq. (58) analytically. There is a growing exponential solution, an algebraically decaying solution, and the physically acceptable exponentially decaying solution given by

$$F(x)=F_\infty \frac{e^{-\mu_0 x^2/2}}{x^{d-\pi/2\mu_0}} . \tag{61}$$

The matching of the short-distance and the physically acceptable long-distance behavior can only be achieved for a selected value for μ. One therefore has a nonlinear eigenvalue problem with $\mu_0=1.104...$ for $d=2$, while $\mu_0=0.5917...$ for $d=3$.

A major accomplishment of the theory [18] is to give good estimates for the nonequilibrium exponent λ [19] characterizing the two-time autocorrelation function

$$\langle \psi(0,t)\psi(0,t')\rangle \sim L^{-\lambda}(t) \tag{62}$$

for $t \gg t'$. The theory gives the relationship

$$\lambda=d-\frac{\pi}{4\mu_0} , \tag{63}$$

and the values obtained for μ_0 and λ from the eigenvalue problem are in good agreement with numerical determinations of λ.

VI. THEORY FOR $A_2 \neq 0$

Consider the theory where averages are over $P[m]$ given by Eq. (23) with all $A_n=0$ except for $n=0$ and 2. We call this the $n=2$ theory. For simplicity, here we restrict the analysis to the case of equal times $t=t_1=t_2$. The final results are presented in terms of the two quantities $f(x)$ and

$$g(x)=\frac{A_2(\mathbf{R}_1-\mathbf{R}_2,t)}{S_0(t)} . \tag{64}$$

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. Since as R goes to 0, f goes to 1, and γ blows up, for consistency, we must eventually choose $g(0)=A_2(11)=0$. Since this result simplifies the subsequent analysis considerably, we enforce this condition at the beginning.

The order-parameter scaling function is related to f and g by

$$F(x)=\frac{2}{\pi}[\sin^{-1}f+2\gamma g] . \tag{65}$$

At the end of Sec. IV, it was suggested 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

$$\langle B(1)\sigma(2)\sigma(3)\cdots\sigma(n+1)\rangle=0 . \tag{66}$$

Here we want to be slightly more ambitious, and in this case where $P[m]$ is characterized by $[C_0, A_2]$ we want to try to enforce essentially all one- and two-point averages of the form

$$\Omega_n(1)=\langle B(1)\sigma^{2n+1}(1)\rangle=0 , \tag{67}$$

$$\Omega^O_{n,l}(12)=\langle B(1)\sigma^{2n}(1)\sigma^{2l+1}(2)\rangle=0 , \tag{68}$$

$$\Omega^E_{n,l}(12)=\langle B(1)\sigma^{2n+1}(1)\sigma^{2l}(2)\rangle=0 , \tag{69}$$

for integers n and l, and the superscripts O and E stand for *odd* and *even* sectors.

In principle, this gives an infinite number of conditions to be satisfied by choosing two functions $[C_0(12), A_2(12)]$. Surprisingly, as we shall see, these can be chosen such that (67) and (69) can be satisfied for all n and l and (68) can be satisfied for $n=l=0$ and is "small" for all other values of n and l.

Let us look first at the condition setting $\Omega_n(1)$ to zero. After minor rearrangements, this can be written in the form

$$\frac{1}{2n+2}\frac{\partial}{\partial t_1}\langle\sigma^{2n+2}(1)\rangle+\frac{1}{2}\langle\sigma_2(1)\sigma^{2n+1}(1)\rangle - \langle\nabla^2\sigma(1)\sigma^{2n+1}(1)\rangle=0 . \tag{70}$$

We are interested in this relation in the long-time large-L limit where we can show, using (42),

$$\langle\sigma^{2n+2}(1)\rangle=\psi_0^{2n+2}+\frac{\kappa_n}{\sqrt{2}L}+O(L^{-3}) , \tag{71}$$

where κ_n is a time-independent integral given by

$$\kappa_n=\int_{-\infty}^{+\infty} dx[\sigma^{2n+2}(x)-\psi_0^{2n+2}] \tag{72}$$

and

$$\langle\sigma_2(1)\sigma^{2n+1}(1)\rangle=\frac{1}{\sqrt{2}L}\kappa_n^{(1)}+0\left[\frac{1}{L^3}\right] , \tag{73}$$

where

$$\kappa_n^{(1)}=\int_{-\infty}^{\infty} dx\,\sigma_2(x)\sigma^{2n+1}(x) . \tag{74}$$

In evaluating the terms depending on the Laplacian of σ, we make use of the local dependence of σ on m to write

$$\nabla^2\sigma=\sigma_2(\nabla m)^2+\sigma_1\nabla^2 m . \tag{75}$$

Using the results reported in the Appendix for evaluating averages over gradients of fields, we obtain, to leading order in L^{-1},

$$\langle\nabla^2\sigma(1)\sigma^{2n+1}(1)\rangle=d_0^{(2)}\frac{1}{\sqrt{2\pi S_0}}\kappa_n^{(1)} , \tag{76}$$

$$d_0^{(2)}=S_0^{(2)}+2A_2^{(2)} , \tag{77}$$

$$S_0^{(2)}=\lim_{\mathbf{R}\to 0}-\nabla_R^2 C_0(\mathbf{R},t) , \tag{78}$$

$$A_2^{(2)}=\lim_{\mathbf{R}\to 0}-\nabla_R^2 A_2(\mathbf{R},t) . \tag{79}$$

Combining all of these results, the n conditions given by (67) reduce to the simple result

$$(\tfrac{1}{2}-d_0^{(2)})\frac{1}{\sqrt{2\pi S_0}}\kappa_n^{(1)}=0 \tag{80}$$

or

$$d_0^{(2)}=\tfrac{1}{2}\ . \tag{81}$$

The condition $\Omega_{n,l}^{O}(12)=0$, in the scaling regime, can be rewritten in the form

$$\frac{\partial}{\partial t}\langle\sigma^{2n+1}(1)\sigma^{2l+1}(2)\rangle = \frac{\psi_0^{2(l+n+1)}}{\pi S_0}\{2\Omega_1+[\kappa_l^{(2)}(2l+1)+\kappa_n^{(2)}(2n+1)]\Omega_2\}\ , \tag{82}$$

where

$$\Omega_1=\gamma(f+2g\gamma^2)+\nabla^2 F\ , \tag{83}$$

$$\Omega_2=2\frac{\gamma^3}{\pi}\{4\pi A_2^{(2)}g+4f\nabla f\cdot\nabla g +(\nabla f)^2[f+2g\gamma^2(1+2f^2)]\}\ , \tag{84}$$

$$\langle\sigma^{2n+1}(1)\sigma^{2l+1}(2)\rangle=\psi_0^{2n+2l+2}F(x)\ , \tag{85}$$

$$\kappa_n^{(2)}=\tfrac{1}{2}\psi_0^{2n+1}\int_{-\infty}^{\infty}dx\,x\sigma_1(x)[\sigma^{2n}(x)]_1\ . \tag{86}$$

Similarly, $\Omega_{n,l}^{E}(12)=0$ takes the form, to lowest order in L^{-1},

$$\left[\frac{2l}{2n+2}\kappa_{l-1,n+1}+\kappa_{n,l}\right]\frac{\gamma^3}{2\pi^2 S_0} \times\{4\pi A_2^{(2)}gf+4\nabla g\cdot\nabla f+(\nabla f)^2(1+6gf\gamma^2)\}=0\ , \tag{87}$$

where

$$\kappa_{n,l}=\kappa_n^{(1)}\kappa_l\ . \tag{88}$$

It is clear that within our current approximation where we have to determine two independent functions f and g we cannot satisfy both sets of equations for all n and l. Instead, we will satisfy (68) for $n=l=0$, (69) for all n and l, and then check to see if Ω_2 is small. Since, to lowest order in L^{-1}, we have from (82), for $n=l=0$,

$$-\mu xF'=f\gamma+2g\gamma^3+\nabla^2 F\ , \tag{89}$$

where $2\Gamma\mu=L\dot{L}$, while (87) becomes, remembering $d_0^{(2)}=\frac{1}{2}$,

$$4\pi A_2^{(2)}gf+4\nabla g\cdot\nabla f+(\nabla f)^2(1+6gf\gamma^2)=0\ . \tag{90}$$

Using this last equation, we can rewrite the expression for Ω_2 in the form

$$\Omega_2=\frac{\gamma^3}{\pi}\{8\pi A_2^{(2)}g+8\pi S_0 g\nabla f\cdot\nabla g +2\pi S_0(\nabla f)^2[f+2g\gamma^2(1+2f^2)]\} =4\frac{\gamma^3}{\pi}g[2\pi A_2^{(2)}(1-f^2)-(\nabla f)^2]\ . \tag{91}$$

While Ω_2 is not zero, it turns out to be small ($|\Omega_2|<0.08$) for all x. It should also be noted here why the conditions $\Omega_1=0$ and $\Omega_{n,l}^{E}=0$ are enforced in the $n=2$ approximation rather than replace one of them with the condition $\Omega_2=0$. The reason is that one can only satisfy $\Omega_2=0$ for large x by choosing $A_2^{(2)}=0$. Clearly, this choice then precludes a nontrivial solution for the eigenvalue problem determining f and g discussed below.

Note, at this point, we have two parameters left in the problem μ and $A_2^{(2)}$. We also have the constraint, since $S_0^{(2)}+2A_2^{(2)}=\frac{1}{2}$ and, since by definition, $S_0^{(2)}\geq 0$, that $A_2^{(2)}\leq\frac{1}{4}$. In our previous work, we found that μ was determined by a nonlinear eigenvalue problem. So also we will find here that $A_2^{(2)}$ is determined as part of a more elaborate nonlinear eigenvalue problem.

For the coupled set of equations, it turns out to be convenient, instead of working with the independent variables f and g, to work with the physical observable F and the quantity

$$H=-\frac{4}{\pi}\gamma g\ . \tag{92}$$

f and g are then given in terms of F and H by

$$f=\sin\left[\frac{\pi}{2}(F+H)\right]\ , \tag{93}$$

$$g=-\frac{\pi}{4}H\cos\left[\frac{\pi}{2}(F+H)\right]\ . \tag{94}$$

In terms of these variables, the basic equations take the form

$$\nabla^2 F+\mu\mathbf{x}\cdot\nabla F(x)+\tan\left[\frac{\pi}{2}(F+H)\right] -\frac{\pi}{2}\frac{H}{\cos^2[(\pi/2)(F+H)]}=0 \tag{95}$$

and

$$\alpha_0^2 qb-2H'(F'+H')+(F'+H')^2(1+b)=0\ , \tag{96}$$

where α_0 is given by (60). It is convenient to introduce the quantity q defined by

$$\alpha_0^2 q=\frac{8A_2^{(2)}}{\pi} \tag{97}$$

and

$$b=-\frac{\pi}{2}H\tan\left[\frac{\pi}{2}(F+H)\right]\ . \tag{98}$$

Equation (96) can be solved for H' to obtain

$$H'=\frac{bF'-\sqrt{(F')^2+\alpha_0^2 qb(1-b)}}{1-b}\ . \tag{99}$$

Again, in the short-distance regime we have an expansion of the form

$$F(x)=1-\alpha x(1+\beta_2 x+\beta_3 x^2+\cdots)\ , \tag{100}$$

where now

$$\alpha=\alpha_0\frac{\sqrt{q(q+2)}}{q+1} \tag{101}$$

and

$$\beta_3=-\frac{q(q+3)}{2}\frac{\mu+(\pi/6)[1+2/(q+2)^2]}{[6(d-1)+3(2d+1)q+(2d+1)q^2]}\ , \tag{102}$$

while H has the expansion

$$H(x)=-h_0x(1+h_2x+h_3x^2+\cdots)\ , \tag{103}$$

where

$$h_0=-\frac{\alpha}{q+2}\ , \tag{104}$$

$h_{\text{even}}=0$, and

$$h_3=\frac{\pi}{6(d-1)}\frac{q(q+1)}{(q+1)^2}+\beta_3\frac{(7q+9)}{(q+3)}\ . \tag{105}$$

We expect for large x that F and H will decay to zero and we find that Eq. (95) reduces to the same linear equation satisfied by F in the Gaussian case. Therefore F for large x is again given by (61), but with μ_0 replaced by μ given by the solution for the coupled set of equations for F and H. Then, since $F'/F\gg1$, one sees that the physical solution for the equation determining H is given by

$$F=H \tag{106}$$

or

$$f=-4g\ . \tag{107}$$

Since for large x we also have

$$f+2g=\frac{\pi}{2}F\ , \tag{108}$$

we can solve for f and g to obtain

$$f=\pi F \tag{109}$$

and

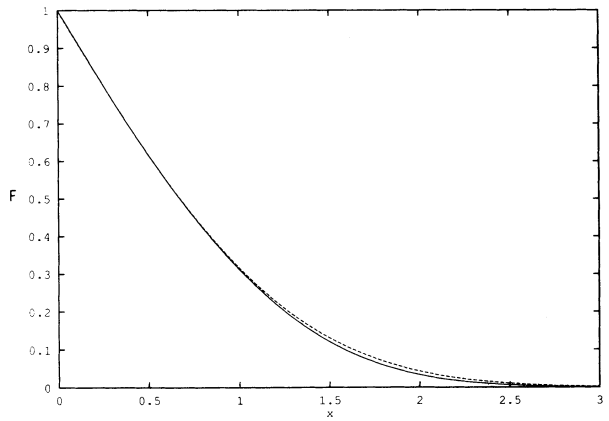

FIG. 1. Scaling function $F(x)$ vs scaled distance x for $d=2$. The dashed line is the Gaussian result, and the solid line is the result for the $n=2$ model.

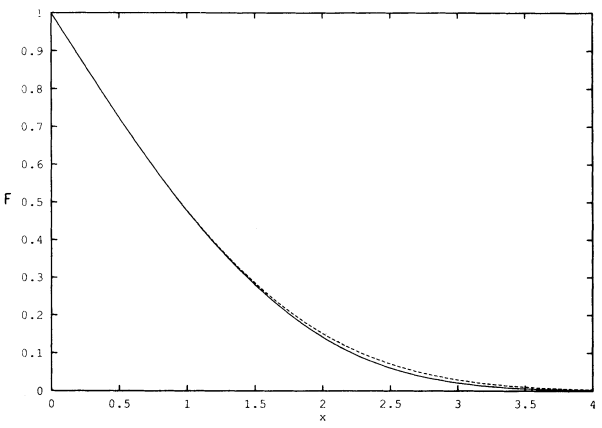

FIG. 2. Scaling function $F(x)$ vs scaled distance x for $d=3$. The dashed line is the Gaussian result, and the solid line is the result for the $n=2$ model.

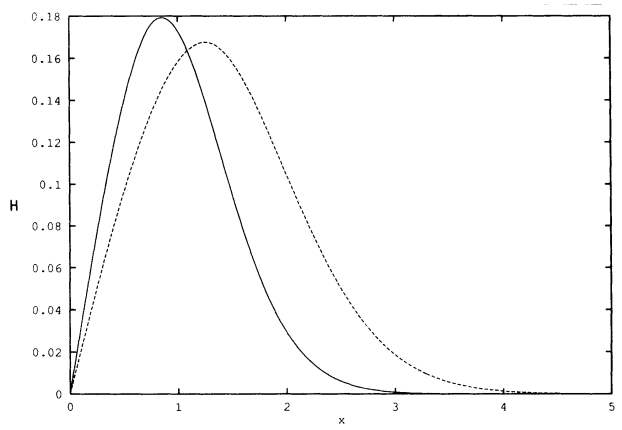

FIG. 3. Function $H(x)$ vs scaled distance x for $d=2$ and 3. The dashed line is the $d=3$ result, and the solid line is the $d=2$ result.

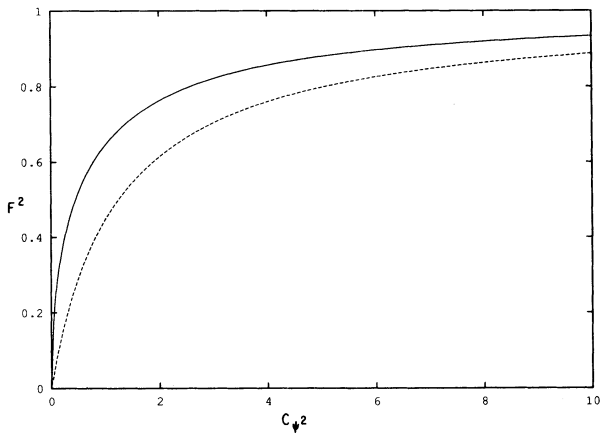

FIG. 4. Higher-order correlation function F^2 vs C_{ψ^2} for $d=2$. The dashed line is the Gaussian result, and the solid line is the result for the $n=2$ model.

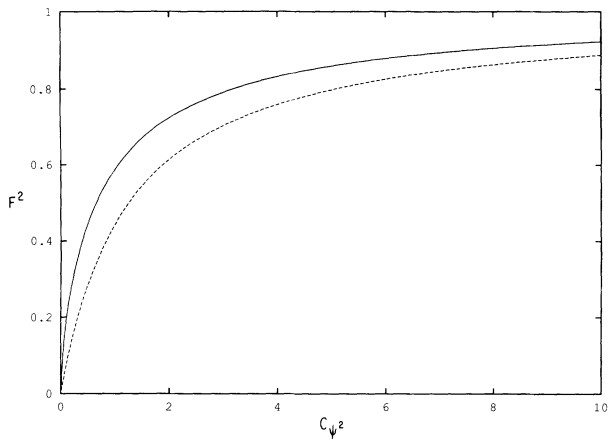

FIG. 5. Higher-order correlation function F^2 vs C_{ψ^2} for $d=3$. The dashed line is the Gaussian result, and the solid line is the result for the $n=2$ model.

$$g=-\frac{\pi}{4}F \ . \tag{110}$$

In this case, in connecting the small- and large-x solutions, we obtain a double-eigenvalue problem for μ and q.

The numerical solution of the coupled set (95) and (99) has several points which require attention. While one must, in a rough sense, choose μ such that F approaches the form (61), one must also be careful to avoid those values of q for which the argument of the square root in (99) is negative. The solution $F=H$ for large x divides two unstable solutions for H. Another technical problem is the matching of the short-distance expressions for H' and F'' resulting from (103) and (100) to those given by (99) and (95).

The scaling functions $F(x)$ and $H(x)$ for $d=2$ are shown in Figs. 1 and 2. The associated eigenvalues are $\mu=0.8271\ldots$ and $q=0.542\,21\ldots$. Also included in Fig. 1 is $F(x)$ found in the Gaussian case. The scaled length in both cases is chosen such that $F(x)=1-\alpha_0 x+\cdots$ for small x. This is equivalent to a change in the growth law from $L(t)$ to $\tilde{L}(t)=(\alpha_0/\alpha)L(t)$. It is clear that the extended theory lies slightly below the Gaussian theory for intermediate values of x. This is clearly in the direction of better agreement with the numerical results as given by Fig. 1 of Ref. [17]. The three-dimensional results for F and H are given in Figs. 3 and 2, respectively. The three-dimensional eigenvalues are given by $\mu=0.519\,80\ldots$ and $q=0.774\,59\ldots$.

It is not difficult to show that the expression relating the nonequilibrium exponent λ to the eigenvalue μ is still given by $\lambda=d-\pi/4\mu$. This follows primarily because, for small F, the terms not involving a gradient in Eq. (95) reduce to $(\pi/2)F$ and are independent of H. Given the new values of μ, we obtain $\lambda=1.050\ldots$ in two dimensions and $\lambda=1.489\ldots$ in three dimensions. Given the numerical results for λ reported in Ref. [8], one sees that the two-dimensional result is now in poorer agreement compared to the Gaussian case, while the three-dimensional value is in somewhat better agreement compared to the Gaussian result.

VII. HIGHER-ORDER QUANTITY C_{ψ^2}

We turn next to the higher-order correlation function C_{ψ^2} defined by Eq. (1). Using the techniques developed above, it is easy to see that within the $n=2$ theory this quantity is given in the scaling regime by

$$C_{\psi^2}=\gamma(1+2gf\gamma^2)-1 \tag{111}$$

or, in terms of the variables F and H,

$$C_{\psi^2}=\frac{1+b}{\cos[(\pi/2)(F+H)]}-1 \ . \tag{112}$$

In the Gaussian approximation, we have

$$C^G_{\psi^2}=\frac{1}{\cos[(\pi/2)F]}-1 \ . \tag{113}$$

For large x, where F is small, this reduces to

$$C^G_{\psi^2}=\frac{\pi^2}{8}F^2 \tag{114}$$

as first obtained by BBS. In the $n=2$ theory, in the large-x limit where both F and H are small, we obtain

$$C_{\psi^2}=\frac{\pi^2}{8}(F^2-H^2) \ . \tag{115}$$

We see then that the observed numerical behavior that C_{ψ^2} goes to zero faster than F^2 occurs only when we satisfy the double-eigenvalue problem which selects $F=H$. We show, in Figs. 4 and 5, F^2 plotted versus C_{ψ^2} as in BBS for two and three dimensions, respectively. While we do not obtain C_{ψ^2} going negative in two dimensions as in the numerical studies, clearly the theory gives much better agreement compared with the Gaussian theory.

VIII. CONCLUSIONS

A more general approach to the theory of growth kinetics, which goes beyond the limitations of the Gaussian approximation for an auxiliary field, has been presented. 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 in the $n=2$ approximation. It is very encouraging that the simple set $\{C_0, A_2\}$ can satisfy almost all of the constraints given by Eqs. (67)–(69). Indeed, one obtains universal forms for $\{C_0/S_0, A_2/S_0\}$ and general improvement in the theory compared to the Gaussian approximation where all $A_n=0$ for $n>0$. It is a bit surprising that the scaling equations determining f and g contain just the two additional parameters μ and $A_2^{(2)}$ needed to satisfy the coupled nonlinear eigenvalue problem.

This success raises a number of intriguing questions. Can one continue to add additional functions $A_4, A_6, \ldots$ and obtain improvement in the theory? If one includes the A_4 term in the analysis, can one satisfy all of the constraints given by Eqs. (67)–(69)? This seems likely. What additional constraints can one then impose? Why do the set of equations labeled by general integers n and l reduce

down to just three independent equations in the scaling regime? Why use the set of moments given by Eqs. (67)–(69) to determine f and g? How can this process be systemized? What is the general structure at work? There is much work to be done in this area.

ACKNOWLEDGMENTS

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APPENDIX

Matrix elements involving gradients for the $n=2$ approximation can be evaluated for general functions of $B[m]$ and $E[m]$ in the form

$$\langle E(1)[\nabla^2 m(1)]B(2)\rangle = -d_0^{(2)}M_{10}+\nabla^2 D_0(12)M_{01}-S_0^{(2)}[A_2^{(0)}(M_{30}+M_{12})+2A_2(12)M_{21}] +\nabla^2 C_0(12)[A_2^{(0)}(M_{21}+M_{03})+2A_2(12)M_{12}] , \tag{A1}$$

where

$$D_0(12)=C_0(12)+2A_2(12) , \tag{A2}$$

$$S_0^{(2)}=-\nabla^2 C_0(12)|_{1\to 2} , \tag{A3}$$

$$d_0^{(2)}=-\nabla^2 D_0(12)|_{1\to 2} , \tag{A4}$$

$$M_{nl}=\langle E_n(1)B_l(2)\rangle_0 , \tag{A5}$$

and

$$A_2^{(0)}=A_2(11) . \tag{A6}$$

Similarly,

$$\langle E(1)(\nabla m)^2 B(2)\rangle = d_0^{(2)}M_{00}+S_0^{(2)}[A_2^{(0)}(M_{20}+M_{02})+2A_2(12)M_{11}]+4\nabla A_2(12)\cdot\nabla C_0(12)M_{02} +[\nabla C_0(12)]^2[M_{02}+A_2^{(0)}M_{22}+2A_2(12)M_{13}+A_2^{(0)}M_{04}] . \tag{A7}$$

The special case where B is a constant gives the one-point quantities

$$\langle E(1)\nabla^2 m(1)\rangle = -d_0^{(2)}\langle E_1\rangle_0 - S_0^{(2)}A_2^{(0)}\langle E_3\rangle_0 , \tag{A8}$$

$$\langle E(1)(\nabla m)^2\rangle = d_0^{(2)}\langle E\rangle_0 + S_0^{(2)}A_2^{(0)}\langle E_2\rangle_0 . \tag{A9}$$

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