Absolute test for theories of phase-ordering dynamics

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Numerical simulation results are presented for phase ordering in the O(n) model with nonconserved order parameter, for $1 \le n \le d$ in dimensions $d=2$ and 3. The two-point correlation functions C_ϕ and C_{ϕ^2} of the order-parameter field and its square are obtained and compared with approximate analytic results obtained by treating the order-parameter field as a function of a Gaussian auxiliary field. Good agreement between theory and simulation is obtained when the functions C_ϕ and C_{ϕ^2} are considered separately, but not when the free parameter of the theory [incorporated in the scaling length $L(t)$] is eliminated by considering the two functions together.

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I. INTRODUCTION

A major goal of the theory of phase-ordering dynamics has been partially fulfilled in recent years by the approximate determination of the scaling function $f(x)$ for the two-point correlation function [1–9], especially for nonconserved fields. Although exact calculations [2] have proved possible only for physically uninteresting values of d and n, the spatial and spin dimensionalities, approximate theories have been proposed [3–5,7–9] which appear to agree closely with simulation results for the two-point correlation function

$$C_\phi(r,t)=\langle \phi(x,t)\phi(x+r,t)\rangle = f_\phi(r/L(t)) \tag{1}$$

and its Fourier transform, the structure factor

$$S_\phi(k,t)=L(t)^d g_\phi(kL(t)) , \tag{2}$$

where $L(t)$ is the characteristic length scale at time t.

In addition, the two-point function of the square of the field

$$C_{\phi^2}(r,t)=\langle \phi^2(x,t)\phi^2(x+r,t)\rangle - \langle \phi^2(x,t)\rangle\langle \phi^2(x+r,t)\rangle \tag{3}$$

has recently been calculated within the framework of these approximate theories [10].

The essential feature of the most successful theories of phase-ordering dynamics is the introduction of an auxiliary field, for which a Gaussian probability distribution is assumed. This field is related to the order-parameter field ϕ by a mapping designed to simplify the time-dependent Ginzburg-Landau (TDGL) equation, the equation of motion for ϕ. Although this approach has been widely used, initially for systems with scalar order parameters [3–6] and later for systems with vector [7–9], and very recently tensor [11], order parameters, the assumption of a Gaussian probability distribution for the auxiliary field has never been directly tested. The purpose of this paper is to use simulation results to determine the accuracy of this approximation.

In the comparison of theoretical predictions with simulation results and experiment it is generally necessary to introduce a free parameter to rescale $L(t)$ because of the different units of time in the TDGL equation and the simulations or experiments. In fact, $L(t)$ is often determined separately at each time t [e.g., by defining $f_\phi(1)=\frac{1}{2}$ in (1)], which amounts to having an adjustable function in the fit. By measuring both C_ϕ and C_{ϕ^2}, however, a direct comparison of theory and simulation can be made by plotting one against the other. Since such a plot contains no free parameters, this approach provides an *absolute* test of the theory. We find that the theoretical results based on the Gaussian approximation, which are independent of the dimensionality d (as far as the relation between C_ϕ and C_{ϕ^2} is concerned), give a rather poor fit to the simulation data, but are closer in $d=3$ than in $d=2$, consistent with the hypothesis that the approximate theory becomes exact for $d\to\infty$ [9]. Note that the test proposed here, involving the correlation functions for ϕ and ϕ^2, provides a necessary, but not sufficient, condition for the correctness of the theory. A *complete* test would require a description of the entire order-parameter distribution, equivalent to testing an infinite number of correlation functions.

II. SIMULATIONS

All the simulations ($d=2,3$; $1\le n\le d$) were performed using cell dynamics, a computationally efficient simulation scheme introduced by Oono and Puri [12]. The essential idea is to take a lattice of "soft" spins, corresponding to a coarse-grained order-parameter field $\boldsymbol{\phi}(r,t)$, and update them with the mapping

$$\boldsymbol{\phi}_{n+1}(i)=D\left[\frac{1}{z}\sum_j \boldsymbol{\phi}_n(j)-\boldsymbol{\phi}_n(i)\right] + E\hat{\boldsymbol{\phi}}_n(i)\tanh(|\boldsymbol{\phi}_n(i)|) , \tag{4}$$

where a caret indicates a unit vector, z is the number of nearest neighbors, and D and E are adjustable parameters, for which we chose the standard values $D=0.5$ and

$E=1.3$ [12].

Previous simulations [13] have measured the conventional two-point correlation function C_ϕ, but not C_{ϕ^2} which we measure here. Equation (3) can be conveniently rewritten as

$$C_{\phi^2}(r,t)=\langle[\phi_0^2-\phi^2(1)][\phi_0^2-\phi^2(2)]\rangle - \langle[\phi_0^2-\phi^2(1)]\rangle\langle[\phi_0^2-\phi^2(2)]\rangle \ , \tag{5}$$

where ϕ_0^2 is the equilibrium value of ϕ^2, which can be obtained from the fixed points of (4), and we have introduced the shorthand "1" for (r_1,t) etc.

It is desirable when measuring C_ϕ to "harden" the fields before calculating the correlation function, i.e., to compute (for general n).

$$C_\phi^H(r,t)=\langle\hat{\boldsymbol{\phi}}(x,t)\cdot\hat{\boldsymbol{\phi}}(x+r,t)\rangle \ , \tag{6}$$

where $\hat{\boldsymbol{\phi}}=\boldsymbol{\phi}/|\boldsymbol{\phi}|$ [for scalar fields $\hat{\phi}=\mathrm{sgn}(\phi)$]. This reduces the effective size of the defects (domain walls, strings, etc.) to zero, enabling scaling to be achieved down to smaller values of r. Unfortunately, the same procedure cannot be applied to C_{ϕ^2} (which would vanish identically for "hard" fields), and hence the scaling for small r is considerably worse in this case.

III. COMPARISON WITH THEORY

For nonconserved fields, the conventional starting point is the TDGL equation

$$\partial_t\boldsymbol{\phi}=\nabla^2\boldsymbol{\phi}-\frac{\partial V}{\partial\boldsymbol{\phi}} \ , \tag{7}$$

where for scalar fields $V(\phi)$ is a symmetric double-well potential with minima at ±1, or a Mexican-hat potential with ground-state manifold $\phi^2=\phi_0^2$ for vector fields. Temperature is an irrelevant variable provided $T<T_c$, so there is no need for a thermal noise term [14]. We consider only the scalar case in detail, as the generalization to vector fields is straightforward.

The two most successful theories of scalar systems, due to Ohta, Jasnow, and Kawasaki (OJK) [4] and Mazenko [5], introduce a spatially smooth auxiliary field $m(r,t)$ which is related to the order-parameter field by a sigmoidal function $\phi=\sigma(m)$ such than an m in the interval $(-\infty,\infty)$ yields a ϕ in the interval $[-1,1]$. By considering the motion of the interfaces, and using a sort of mean-field theory to make the equation of motion for m isotropic, OJK obtain the diffusion equation

$$\frac{\partial m}{\partial t}=D\nabla^2 m \ , \tag{8}$$

where $D=(d-1)/d$. A similar equation was derived by Kawasaki, Yalabik, and Gunton (KYG) [3] using a singular-perturbation-theory approach. At late times, ϕ has one of the values ±1 almost everywhere and, as far as the calculation of C_ϕ is concerned, one can set $\phi=\mathrm{sgn}(m)$ in the scaling regime. If the initial conditions for m have only short-range Gaussian correlations, this Gaussian property continues to all times, as (8) is linear. The general Gaussian form for the joint probability distribution of $m(1)$ and $m(2)$ is

$$P(m(1),m(2))=N\exp\left[-\frac{1}{2(1-\gamma^2)}\times\left[\frac{m(1)^2}{S_0(1)}+\frac{m(2)^2}{S_0(2)}-\frac{2\gamma m(1)m(2)}{\sqrt{S_0(1)S_0(2)}}\right]\right] , \tag{9}$$

where

$$S_0(1)=\langle m(1)^2\rangle,\ S_0(2)=\langle m(2)^2\rangle \ , \tag{10}$$

$$\gamma=\frac{\langle m(1)m(2)\rangle}{\sqrt{S_0(1)S_0(2)}},\quad N=\frac{1}{2\pi\sqrt{(1-\gamma^2)S_0(1)S_0(2)}} \ .$$

The correlation function

$$C_\phi(r,t)=\langle\phi(1)\phi(2)\rangle=\langle\mathrm{sgn}(m(1))\mathrm{sgn}(m(2))\rangle \tag{11}$$

can be evaluated to give

$$C_\phi(r,t)=\frac{2}{\pi}\sin^{-1}(\gamma) \ , \tag{12}$$

where in the OJK theory $\gamma=\exp(-x^2/8)$ and $x=r/\sqrt{Dt}$. For vector fields, $C_\phi=\langle\hat{\mathbf{m}}(1)\cdot\hat{\mathbf{m}}(2)\rangle$ instead. Using the distribution (9) separately for each component (since $\mathbf{m}$ is taken to be a Gaussian field) gives [7–9]

$$C_\phi(r,t)=\frac{n\gamma}{2\pi}\left[B\left[\frac{n+1}{2},\frac{1}{2}\right]\right]^2 F\left[\frac{1}{2},\frac{1}{2};\frac{n+2}{2};\gamma^2\right], \tag{13}$$

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

These expressions are independent of the relation between γ and the scaling variable x. In the Mazenko approach, the only assumption is that $P(m(1),m(2))$ has the Gaussian form (9), which gives (12) [or (13) for vector fields] immediately. By choosing the relation between ϕ and m to be the equation for an equilibrium domain wall (or, for vector fields, the appropriate topological defect [8,9]), m can be regarded as a coordinate measuring the distance from a domain wall (or other defect). A self-consistent equation for the correlation function in terms of the scaling variable x can then be derived for scalar fields [5]. For vector fields there is no closed form for $C_\phi(x)$, but an equation for $\gamma(x)$ can be solved numerically and the solution inserted into (13) to obtain $C_\phi(x)$ [8,9].

Using the same Gaussian assumption, the evaluation of C_{ϕ^2} in terms of γ is straightforward [10]. For general n (with $\phi_0^2=1$),

$$\langle[1-\phi^2(1)][1-\phi^2(2)]\rangle=\int d\mathbf{m}(1)\int d\mathbf{m}(2)P(\mathbf{m}(1),\mathbf{m}(2))[1-\phi^2(\mathbf{m}(1))][1-\phi^2(\mathbf{m}(2))] \ . \tag{14}$$

For scalar fields, $\phi(m)$ approaches ± 1 exponentially fast as $m \to \pm\infty$, whereas $P(m(1),m(2))$ is slowly varying function of $m(1)$ and $m(2)$ [varying on the scale $L(t)$]. It follows that for late times the integral is dominated by points close to $m(1)=0$, $m(2)=0$, and hence can be evaluated as

$$\langle [1-\phi^2(1)][1-\phi^2(2)]\rangle = \left[\int dm\,[1-\phi^2(m)]\right]^2 P(0,0)\ , \tag{15}$$

where $P(0,0)$ follows from Eq. (9). If this result is normalized by $\langle [1-\phi^2(1)]\rangle\langle [1-\phi^2(2)]\rangle$ then the normalized, connected correlation function is [10]

$$C^N_{\phi^2} = \frac{\langle [1-\phi^2(1)][1-\phi^2(2)]\rangle}{\langle [1-\phi^2(1)]\rangle\langle [1-\phi^2(2)]\rangle} - 1 = \frac{1}{\sqrt{1-\gamma^2}} - 1\ . \tag{16}$$

For vector fields the calculation is more complicated because the function $\boldsymbol{\phi}(\mathbf{m})$ approached $\hat{m}$ as $1/|\mathbf{m}|^2$, rather than as an exponential [8]. The integral (14) can still be done, however, giving the result for C_{ϕ^2}, normalized by its large distance behavior, as [10]

$$C^N_{\phi^2} = \frac{\langle [1-\phi^2(1)][1-\phi^2(2)]\rangle}{\langle [1-\phi^2(1)]\rangle\langle [1-\phi^2(2)]\rangle} - 1 = F(1,1;n/2;\gamma^2) - 1,\quad n \geq 2\ . \tag{17}$$

The dependence of γ on the scaling variable x is the same as for C_ϕ, since γ enters only through the probability distribution (9). The hypergeometric function in (17) simplifies for the integer n values of physical interest, becoming simply $1/(1-\gamma^2)$ for $n=2$, and $\sin^{-1}(\gamma)/\gamma\sqrt{1-\gamma^2}$ for $n=3$. For $n=2$, the integrals in (14) are logarithmically divergent at small $|\mathbf{m}|$, and hence a cutoff has to be introduced, corresponding to the defect core size [10]. The result obtained reduces to (17) in the scaling limit ($r \to \infty$, $L \to \infty$, with r/L fixed), although the corrections to scaling are of order $1/\ln(L/a)$, where L is the domain scale and a the defect core size, and hence the crossover to the scaling regime is only very slow.

A direct comparison of these results with cell dynamics of Monte Carlo simulations is not possible because of the different time scale in the TDGL equation, which is related to the simulation time scale by a rescaling $t=\alpha t'$. The parameter α is usually chosen so that the best fit between the theoretical predictions and the simulation results is obtained. Unfortunately, this has the effect of introducing a free parameter in the theory and, as the forms of the correlation functions are somewhat featureless, it is perhaps not too surprising that a rather good fit can be found.

The free parameter α can be removed by plotting $(C^H_\phi)^2$ against $C^N_{\phi^2}$ as shown in Figs. 1–5. We plot $(C^H_\phi)^2$, rather than C^H_ϕ, in order to expand the scale near the origin, which corresponds to $\gamma=0$ (or large values of the scaling variable x). Also, since (13) and (17) imply $C_\phi \sim \gamma$ and $C_{\phi^2} \sim \gamma^2$ for $\gamma \to 0$, the Gaussian approximation predicts that the plots of $(C^H_\phi)^2$ against $C^N_{\phi^2}$ should be linear near the origin. Each data point represents a measurement of C^H_ϕ and $C^N_{\phi^2}$ at the same time t and separation r. The data for values of C^H_ϕ close to unity, corresponding to small x, do not scale because, as we mentioned above, the spins could not be hardened in the calculation of $C^N_{\phi^2}$. The data for the earliest time depart for the scaling curve first, as they correspond to the smallest values of r for a given $x=r/L(t)$. The true scaling curve is closest to the late time data, and forms an envelope curve to which the data at progressively later times cross over. Note that we have not had to make any assumption about the form of the scaling to obtain this collapse of the data. That the data collapse onto a universal curve shows that the system is in the scaling regime.

The continuous curves in Figs. 1–5 represent the theoretical forms for C^H_ϕ and $C^N_{\phi^2}$ parametrized by γ. [For the scalar theory, γ can be explicitly eliminated between (12) and (16) to give $C^N_{\phi^2}=\sec(\pi C_\phi/2)-1$.] The Mazenko and OJK theories give the same curves because they differ only in the relationship between γ and the scaling variable x. By plotting the data in this way, therefore, we are directly testing the Gaussian approximation made in the theories, which clearly is poor as none of the curves fit the data at all well. They do not even have the predicted linear behavior at small C_ϕ (i.e., near the origin in Figs. 1–5, corresponding to *large* distances). In fact, for the $d=2$ scalar theory $C^N_{\phi^2}$ is negative at small C_ϕ. Although the values are quite close to zero, the data scale well in this region so we have no reason to expect that it is not a real effect. A similar, though less pronounced, effect is suggested by the data in Fig. 3. This rather interesting feature, which appears to be confined to $d=2$, is not captured by the Gaussian

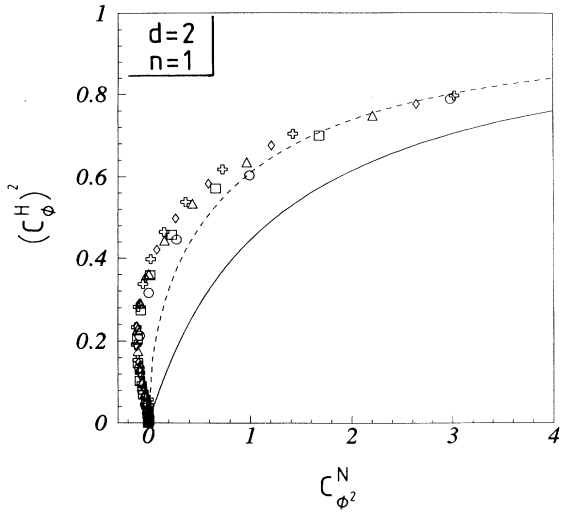

FIG. 1. Plot of $(C^H_\phi)^2$ against $C^N_{\phi^2}$ for the $d=2$ scalar system. The data were averaged over 30 histories of a 700^2 lattice. The circles, squares, triangles, diamonds, and crosses represent data at times 400, 800, 1200, 1600, and 2000 steps, respectively. The continuous curve is the theoretical prediction; the broken curve is the result of fitting $C^N_{\phi^2}$ and C^H_ϕ independently to the theory, as described in the text.

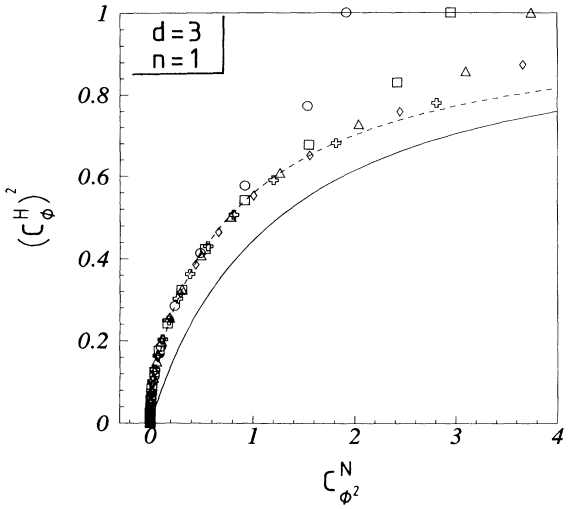

FIG. 2. Same as Fig. 1, but for the $d=3$ scalar system. The data were averaged over 45 histories of an 80^3 lattice. The circles, squares, triangles, diamonds, and crosses represent data at times 100, 200, 300, 400, and 500 steps, respectively. The continuous and broken curves have the same meanings as in Fig. 1.

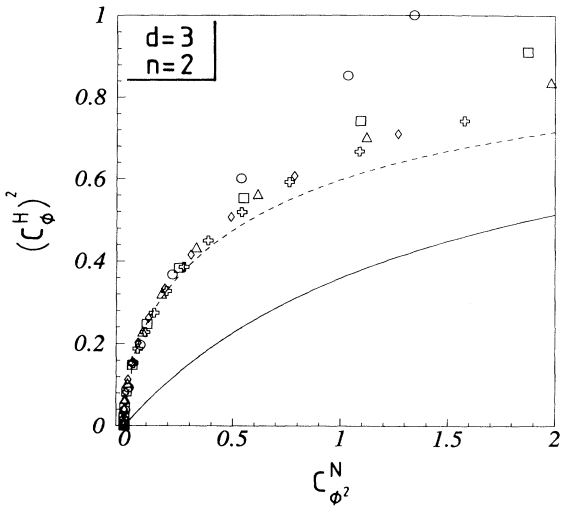

FIG. 4. Same as Fig. 1, but for the $d=3$ O(2) model. The data were averaged over 250 histories of a 64^3 lattice. The circles, squares, triangles, diamonds, and crosses represent data at times 40, 80, 160, 320, and 640 steps, respectively.

theories at all. It is interesting to note, however, that for both $n=1$ and 2 the data lie closer to the theoretical curves (which are d independent) for $d=3$ than for $d=2$. This improvement is consistent with the hypothesis that the Gaussian approximation becomes exact for $d\to\infty$ [9,15].

It should be noted that only data corresponding to correlations along lattice axes are presented in Figs. 1–5. With one exception, the data for correlations along lattice diagonals were found to be indistinguishable from that for the lattice axes, suggesting that the correlation functions are isotropic. The exception is the case $d=2$, $n=1$, where the C_{ϕ^2} data for diagonals seem to lie on a separate scaling curve close to, but distinct from, the lattice axis data (with $C^N_{\phi^2}$ still negative for small C_ϕ). We do not fully understand this, but suspect it may be due to some anistropy in the *internal structure* of the individual domain walls (as opposed to their *global morphology),* associated with the use of a finite grid for the simulation. Note that, for scalar fields, C_{ϕ^2} probes the walls themselves, since $(1-\phi^2)$ is essentially the wall density, while C_ϕ is sensitive only to the global morphology, and insensitive to the internal structure of the wall.

It is surprising, considering how poorly the data are fitted, that both C^H_ϕ and $C^N_{\phi^2}$ are in general rather close to the theoretical functions when considered separately. We have determined the length scale $L(t)$ needed to scale the

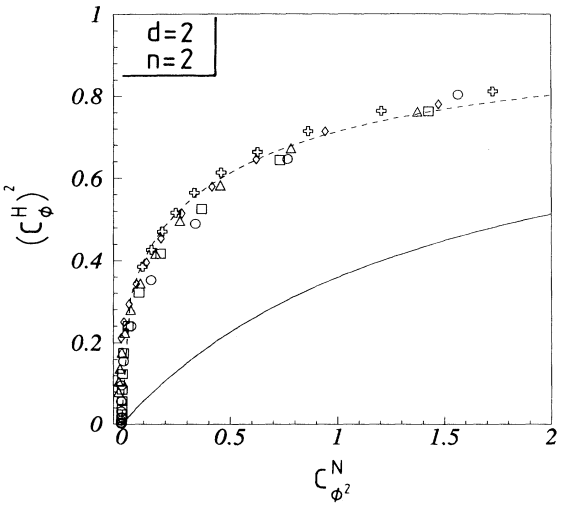

FIG. 3. Same as Fig. 1, but for the $d=2$ O(2) model. The data were averaged over 500 histories of a 128^2 lattice. The circles, squares, triangles, diamonds, and crosses represent data at times 80, 160, 320, 640, and 1280 steps, respectively.

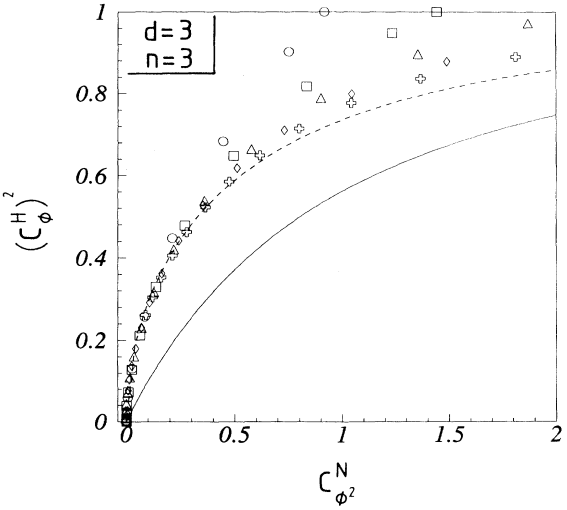

FIG. 5. Same as Fig. 1, but for the $d=3$ O(3) model. The data were averaged over 50 histories of a 64^3 lattice. The circles, squares, triangles, diamonds, and crosses represent data at times 40, 80, 160, 320, and 640 steps, respectively.

data by fitting the simulation results to the theoretical functions. Of course, the $L(t)$ for C_ϕ^H and $C_{\phi^2}^N$ differ by a multiplicative factor but the resulting fits are rather good. We take $\gamma=\exp(-x^2/8)$ for $C_{\phi^2}^N$ and $\gamma=\exp(-k^2x^2/8)$ for C_ϕ^H, where x is the scaling variable and k is a free parameter. These choices correspond to the use of OJK-type theories for C_ϕ and C_{ϕ^2} [4,10]. The broken curves in Figs. 1–5 represent the best fit by eye to the data using this free parameter. The corresponding values of k, written $k(n,d)$, are $k(1,2)=0.65$, $k(1,3)=0.75$, $k(2,2)=0.50$, $k(2,3)=0.65$, and $k(3,3)=0.70$. With the exception of the $d=2$, $n=1$ data (Fig. 1), the resulting fits are quite reasonable. Note that, for given n, k is larger for $d=3$ than for $d=2$, consistent with the notion [9,15] that it approaches unity for large d. As might be expected, the $d=2$ curves are not fitted as well as the $d=3$ curves, which were closer to the theoretical predictions before the introduction of the free parameter.

IV. DISCUSSION AND SUMMARY

We have performed numerical simulations of the O(n) model for $1\leq n\leq d$ in dimensions $d=2$ and 3. The general *forms* obtained for the correlation functions C_ϕ and C_{ϕ^2} agree reasonably well with the predictions of the theories of OJK and Mazenko and their extensions. By plotting $(C_\phi^H)^2$ against $C_{\phi^2}^N$ we have eliminated any adjustable parameters from the theory, and also removed the need for a relation between γ and the scaling variable x, hence directly testing the validity of the Gaussian approximation. Our data do not agree well with the calculated curves, although they are closer for the larger values of d. If it proves possible to calculate systematic corrections to the Gaussian theories [16], our method of examining the results should prove to be a sensitive test of their accuracy.

It would be interesting to apply the same method of systems with random bonds. Simulations of disordered scalar systems in $d=2$ [17,18] found that the two-point correlation function seems to be indistinguishable from that of the pure system, suggesting that (despite the different growth laws [17–19]) pure and disordered systems belong to the same universality class for phase ordering [20]. To make the comparison the usual rescaling of lengths, by a length scale $L(t)$ determined from the data, was required. The same choice of $L(t)$, however, fitted both equal-time and two-time correlation functions [17], providing further support for universality. The present method of calculating C_ϕ and C_{ϕ^2} simultaneously, and plotting one against the other [thus eliminating $L(t)$ altogether], would provide an additional, and more exacting, test.

Note added in proof. The Gaussian assumption for the auxiliary field m is examined critically in recent work by Yeung, Oono, and Shinozaki. Like us, they conclude that the Gaussian approximation is not quantitatively accurate.

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