

## Ordering kinetics of conserved $XY$ models

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The zero-temperature ordering kinetics of conserved  $XY$  models in spatial dimensions  $d = 2$  and  $3$  is studied using cell dynamical simulations. The growth of the characteristic length scale  $L(t)$  is fully consistent with recent theoretical predictions:  $L(t) \sim t^{1/4}$  for  $d = 2$  and  $L(t) \sim (t \ln t)^{1/4}$  for  $d = 3$ . A Gaussian closure approximation describes the form of the structure factor rather well for  $d = 3$ .

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Recently, there has been considerable interest in the kinetics of phase ordering in systems described by non-scalar order parameters [1]. The two fundamental questions usually addressed are (a) the extent to which the familiar scaling phenomenology, developed in the context of scalar systems [2], is applicable to nonscalar systems and (b) if scaling holds, the nature of the growth law for the characteristic scale  $L(t)$  that describes the coarsening dynamics,  $t$  being the time.

In recent work, Bray and Rutenberg (BR) have addressed the second of these questions using an “energy scaling” argument [3]. They obtain predictions for the asymptotic form of  $L(t)$  for all systems for which scaling holds and for which the dynamic is purely dissipative.

The simplest nonscalar systems are  $XY$  models [or  $O(2)$  systems]. There have been a number of recent simulations of the ordering kinetics of  $XY$  systems, for both nonconserved [4, 5] and conserved [6, 7] dynamics, and some experimental studies of related liquid crystal systems [8]. For nonconserved dynamics, the growth laws predicted by BR are  $L(t) \sim (t/\ln t)^{1/2}$  for  $d = 2$  and  $L(t) \sim t^{1/2}$  for  $d \geq 3$  (see also the related work by Yurke *et al.* [9]), provided scaling holds. For conserved dynamics, the corresponding predictions are [3]  $L(t) \sim t^{1/4}$  for  $d = 2$  and  $L(t) \sim (t \ln t)^{1/4}$  for  $d \geq 3$ .

The present work has two goals. First, we present numerical results from an extensive cell dynamical system (CDS) [10] study of phase ordering dynamics for the conserved  $XY$  model for  $d = 2$  and  $3$ . In contrast to previous numerical works, we present data for the “hardened structure factor,” enabling a clear observation of the generalized Porod tail behavior [11]. Our results unambiguously demonstrate dynamical scaling for both  $d = 2$  and  $d = 3$  and are consistent with the theoretical predictions for  $L(t)$ . In particular, there is clear evidence for the predicted logarithmic correction to power-law growth for  $d = 3$ .

The second goal of this study is to examine the utility of Gaussian closure schemes in computing the analytic form of the time-dependent structure factor. Our analytic results using a Gaussian closure scheme are in reasonable agreement with the numerical data for  $d = 3$ , but do not show good agreement with the data for  $d = 2$ . This suggests that, as is known to be true in the non-conserved case [5, 12], Gaussian closure schemes for the conserved case may be better for higher dimensionality. It should be noted, however, that the Gaussian closure scheme, at least in the simple form employed here, fails to capture the predicted logarithmic correction to  $t^{1/4}$  growth for the  $O(2)$  model in  $d > 2$ . In some sense, the  $t^{1/4}$  growth is “built into” the scheme through the naive dimensions of the time and space derivatives in the equation of motion. A similar problem is encountered when applying this approach to the conserved scalar system, when a naive application produces  $t^{1/4}$  growth instead of the correct  $t^{1/3}$  growth [13]. This deficiency can be overcome, but only at the cost of further uncontrolled approximations [13, 14].

The dynamical equation (in dimensionless form) for the ordering of the conserved  $XY$  model has the form

$$\partial_t \vec{\phi} = -\nabla^2 [\nabla^2 \vec{\phi} - \partial V / \partial \vec{\phi}], \quad (1)$$

where  $\vec{\phi}$  is a two-component vector order parameter and  $V(\vec{\phi})$  has a Mexican hat form, e.g.,  $V(\vec{\phi}) = (1 - \vec{\phi}^2)^2$ , with a degenerate manifold of ground states,  $|\vec{\phi}| = 1$ . The CDS models used in our simulations were obtained by a conventional Euler discretization of (1) using an isotropic discrete Laplacian. The mesh sizes of our discretization were so large that it would be incorrect to claim that the solution of our numerical scheme accurately shadows that of the original partial differential equation. Thus our models are justifiable only as CDS models belonging to the same dynamical universality class as the underlying partial differential equation [10]. Our  $d = 2$  simulations were carried out on lattices of size  $256^2$  (with mesh sizes  $\Delta t = 0.15$  and  $\Delta x = 1.7$ ) and the spherically averaged structure factor was computed as an average over 80 runs with independent random initial conditions. Our  $d = 3$  simulations were carried out on lattices of size  $64^3$  (with

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mesh sizes  $\Delta t = 0.1$  and  $\Delta x = 1.7$ ) and the structure factor was calculated as an average over 50 independent runs. The data were “hardened,” i.e., the structure factor was computed using fields renormalized to the length obtained from the fixed points of the CDS iteration scheme. This procedure gives better scaling at large momenta and elucidates the asymptotic tail behavior, which can be masked at late times by finite defect sizes [15]. If scaling is valid, the spherically averaged structure factor  $S(k, t)$  takes the scaling form  $S(k, t) = L^d g(kL)$ , where  $L = L(t)$  is the characteristic scale at time  $t$  and  $g(x)$  is a universal scaling function. The length  $L(t)$  was defined in the usual way to be the reciprocal of the first moment  $\langle k \rangle$  of the structure factor, i.e.,  $L(t) = \langle k \rangle^{-1}$ , where  $\langle k \rangle = m_1/m_0$ , and the  $m_n$  are the “moments” of the structure factor  $m_n = \int_0^\infty dk k^n S(k, t)$ . In this way, the length scale  $L(t)$  is extracted directly from the structure factor data.

The scaled structure factor data are shown in Figs. 1 ( $d = 3$ ) and 2 ( $d = 2$ ) in (a) linear-linear and (b) log-log form. The data collapse is good for both systems. The log-log plots reveal the large- and small- $x$  behavior of the scaling function  $g(x)$ . The large- $x$  behavior follows the predicted power-law form [11]  $g(x) \sim x^{-(d+2)}$  (“generalized Porod law”), which is a consequence of the vortex ( $d = 2$ ) or vortex-line ( $d = 3$ ) topological defects present in the system [16]. The continuous curves, which are obtained from the approximate analytical treatment discussed shortly, have this feature built in and thereby serve as useful guides to the eye in the large- $x$  regime. There is a hump in the log-log plots of Figs. 1(b) and 2(b) at  $x \approx 3$ . This is more clearly seen in the “Porod plot” of  $g(x) x^{d+2}$  against  $x$  (which we plan to present elsewhere) and is reminiscent of the hump in the struc-

ture factor for the conserved scalar case [17]. For small  $x$ , the data are consistent with the expected  $x^4$  behavior (broken lines), which can be derived [1] using an extension of the method used to obtain the  $x^4$  behavior for scalar systems [18].

The results for  $L(t) = \langle k \rangle^{-1}$  are presented in Fig. 3. In both cases ( $d = 2, 3$ ) we attempt two different fits: a simple power-law fit  $L(t) = At^x$  [Fig. 3(a)] and a power-law corrected by a logarithm  $L(t) = A[t \ln(t/\tau)]^x$  [Figure 3(b)]. The values of the best-fit exponent  $x$  in each case and the time scale  $\tau$  for the logarithmic fits are shown on the figure. For  $d = 3$ , the logarithmic fit is extremely good and much better than a simple power law. The best-fit exponent  $x = 0.250$  is in perfect agreement with BR’s prediction  $x = 1/4$ . When a simple power law is forced through the  $d = 3$  data, the fit is much poorer than with the logarithmic correction and the value of  $x$  (0.30) is unreasonably large. By contrast, for the  $d = 2$  data a simple power law gives a good fit (much better than for  $d = 3$ ), with a best-fit exponent  $x = 0.247$ , again pleasingly close to the theoretical prediction  $x = 1/4$ . The logarithmic fit also works acceptably well for this case (as the presence of an additional fitting parameter, i.e.,  $\tau$ , would lead us to expect), but the corresponding value of  $x$  (0.21) is unreasonably small. We conclude that the data for both dimensionalities are completely consistent with BR’s prediction. Of course, it is possible that other fitting functions might fit equally well. We regard it as significant, however, that fitting functions motivated by BR’s predictions yielded fitted exponents in precise agreement with BR’s predictions.

Previous studies of the conserved XY model in  $d = 2$  by Mondello and Goldenfeld [6] also found  $L(t) \sim t^{0.25}$ ,

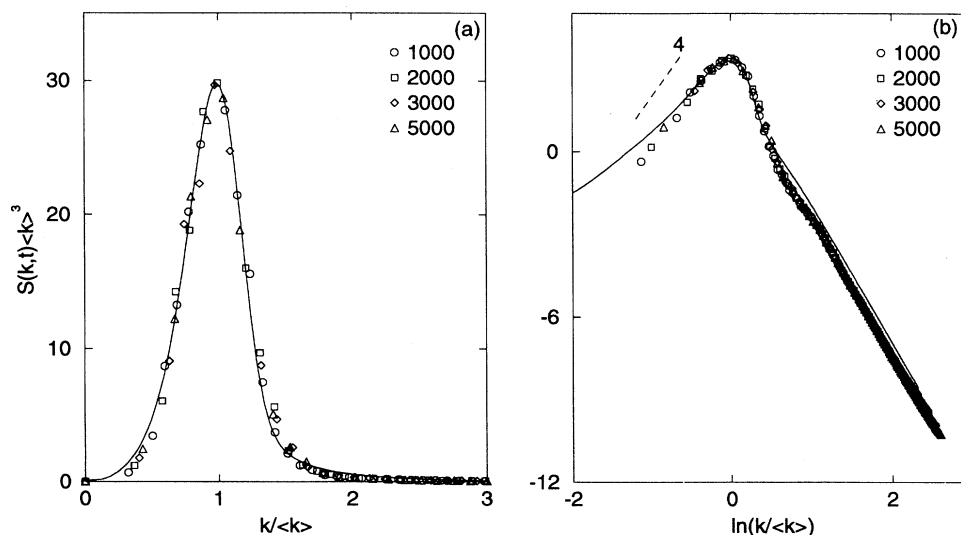


FIG. 1. Scaled structure factor for  $d = 3$ : (a) linear-linear plot and (b) log-log plot. The data are for dimensionless times 1000, 2000, 3000, and 5000, as indicated. Details of the simulation are described in the text. The continuous curves are the numerical Fourier transforms of the scaling function for the pair correlation function, calculated using the Gaussian closure scheme described in the text. The dashed line in (b) has slope 4.

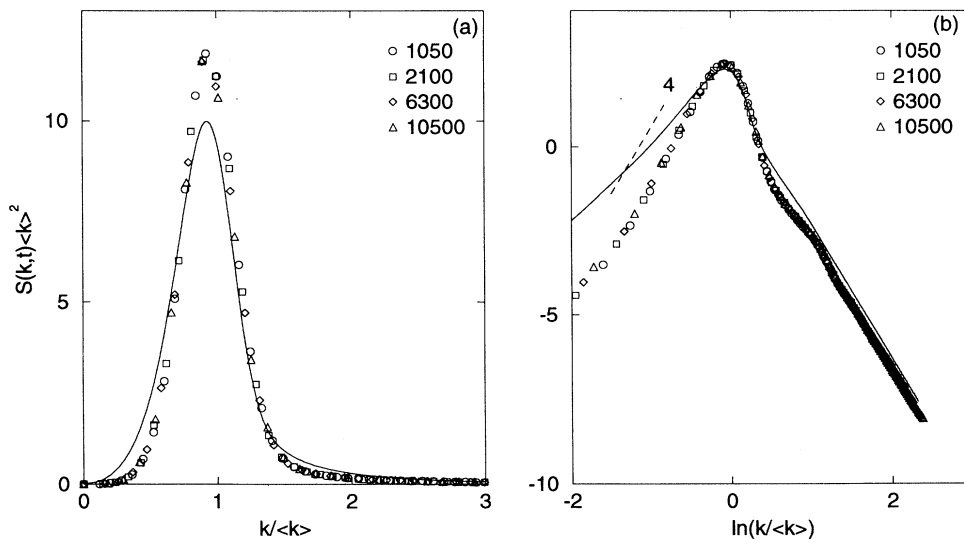


FIG. 2. Same as Fig. 2, but for  $d = 2$ . Here the data are for dimensionless times 1050, 2100, 6300, and 10 500.

but there was some evidence for weak scaling violations: it was not possible to simultaneously collapse both the position and height of the peak in  $S(k, t)$ . Of course, we should point out that the results presented in [6] had a substantially larger dynamic range (about 2.3 decades in  $t$ ) than those in Fig. 2 (one decade in  $t$ ). However, the data in [6] exhibit weak scaling violations even over dynamic ranges comparable with ours. Apart from this, we note that our statistics (average over 80 runs) are somewhat better than those of Mondello and Goldenfeld (40 runs) and that their data were not hardened. However, is not clear to us that either of these facts should cause such an appreciable improvement around the peak

position. In this context it is worth noting that recent studies [5] of the *nonconserved* XY model in  $d = 2$  found evidence for strong scaling violations when the characteristic spacing between vortices,  $d(t) = \rho^{-1/2}$  with  $\rho$  being the vortex density, was used as the scaling length  $L(t)$ . It would be interesting to carry out a similar study for the conserved case (the vortex density was not measured in the present simulations).

Previous simulations for  $d = 3$  conserved XY systems [7], on smaller systems ( $48^3$ ) than those studied here, were originally interpreted in terms of power-law growth  $L(t) \sim t^x$ . For  $T = 0$ , the value  $x \simeq 0.29$  was obtained, close to the value  $x \simeq 0.30$  obtained here with a sim-

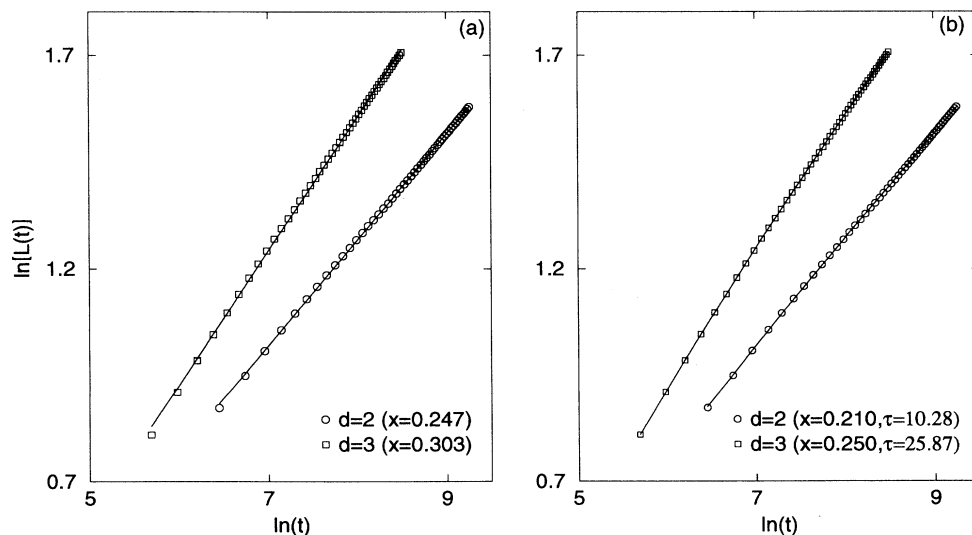


FIG. 3. Growth of the characteristic length scale  $L(t)$  for the conserved XY model, fitting to (a)  $L(t) = At^x$  and (b)  $L(t) = A(t \ln[t/\tau])^x$ . The best-fit values of  $x$  and  $\tau$  are specified on the figures.

ple power law fit, but the quality of the fit was not very good. Subsequently, Siegert has shown that the logarithmic form proposed by BR (with exponent 1/4) gives a very good fit [19]. Some simulations at  $T > 0$  were fitted to a power law with  $x \simeq 0.26$ , but again the logarithmic form (with exponent 1/4) gives a much better fit (but with a different  $\tau$  than for  $T = 0$ ) [19].

We turn now to our approximate analytical treatment, based on a ‘‘Gaussian closure approximation’’ applied to the equation of motion. This approach requires a straightforward modification of equivalent treatments of nonconserved  $n$ -vector fields [20], which in turn generalize an earlier treatment of nonconserved scalar fields [21]. Here we just sketch the derivation and obtain results for the conserved  $XY$  model ( $n = 2$ ). A fuller treatment, with applications to other values of  $n$ , is planned to be given in a longer paper [22]. The starting point is the extension (1) of the Cahn-Hilliard equation [1] to vector fields. The first step is to take the scalar product of (1), evaluated at space-time point 1, with  $\vec{\phi}(2)$ , the field at space-time point 2, and average over an ensemble of initial conditions. This gives

$$\partial_{t_1} C(12) = -\nabla^2 [\nabla^2 C(12) - \langle \vec{\phi}(2) \cdot \partial V / \partial \vec{\phi}(1) \rangle], \quad (2)$$

where  $C(12) \equiv \langle \vec{\phi}(1) \cdot \vec{\phi}(2) \rangle$  is the pair correlation function. In deriving (2), we exploited the translational invariance of the ensemble of initial conditions. Following earlier studies of nonconserved systems [20], we impose an approximate closure of the exact equation (2) through a Gaussian assumption for an auxiliary vector field  $\vec{m}(\mathbf{x}, t)$ , related to the physical field  $\vec{\phi}$  via through the equation

$$\nabla_m^2 \vec{\phi} = \partial V / \partial \vec{\phi} \quad (3)$$

for the function  $\vec{\phi}(\vec{m})$ . Equation (3) is to be solved with boundary conditions  $\vec{\phi}(\vec{0}) = \vec{0}$ ,  $\vec{\phi}(\vec{m}) \rightarrow \hat{m}$  for  $|\vec{m}| \rightarrow \infty$ , where  $\hat{m} = \vec{m}/|\vec{m}|$  is a unit vector. The Laplacian operator in Eq. (3) is defined by  $\nabla_m^2 \equiv \sum_{i=1}^n \partial^2 / \partial m_i^2$ , where the  $m_i$ 's are the Cartesian components of the vector  $\vec{m}$ . The physical meaning of (3) is that the function  $\vec{\phi}(\vec{m})$  gives the structure of an equilibrium defect, with  $|\vec{m}|$  regarded as the distance from the defect core [20].

The key approximation here is to treat  $\vec{m}$  as a Gaussian random field in (2). For nonconserved fields, this approximation is qualitatively accurate and becomes quantitatively accurate with increasing  $d$  [1, 12]. For conserved fields its status is less clear, but it provides a useful starting point for the discussion of scaling functions for conserved vector fields. [We remind the reader that the Gaussian approximation in its present form is not even a reasonable starting point for conserved *scalar* systems, which have an altogether different growth law, i.e.,  $L(t) \sim t^{1/3}$ , than the conserved vector case.] Using (3) to eliminate the explicit dependence on the potential in (2), and exploiting the Gaussian property, we obtain a closed equation for  $C(12)$ . For equal-time correlations, this reads

$$\frac{1}{2} \frac{\partial C}{\partial t} = -\nabla^2 \left[ \nabla^2 C + \frac{1}{\langle m^2 \rangle} \gamma \frac{dC}{d\gamma} \right]. \quad (4)$$

In (4)  $\langle m^2 \rangle$  is the variance of *one* component  $m$  of  $\vec{m}$ ,  $\gamma = \langle m(1)m(2) \rangle / \langle m^2 \rangle$  is the normalized correlator of  $m$ , and the function  $C(\gamma)$  for general  $n$  is given by [11, 20]

$$C(\gamma) = \frac{n\gamma}{2\pi} \left[ B \left( \frac{n+1}{2}, \frac{1}{2} \right) \right]^2 {}_2F_1 \left( \frac{1}{2}, \frac{1}{2}; \frac{n+2}{2}; \gamma^2 \right), \quad (5)$$

where  $B(x, y)$  is the beta function and  ${}_2F_1(a, b; c; z)$  is the hypergeometric function.

The next step is to seek a scaling solution  $C = f(r/L)$ , in which all the time dependence is contained in  $L = L(t)$ . Requiring that all terms in (5) scale in the same way forces  $\langle m^2 \rangle = \alpha L^2$  and  $L = (8t)^{1/4}$  (where the factor 8 is put in for convenience). Recasting (4) as an equation for  $\gamma(x)$ , where  $x = r/L$  is the scaling variable, gives

$$\frac{1}{f_\gamma} \nabla_x^{-2} (f_\gamma x \gamma') = \nabla_x^2 \gamma + \alpha \gamma + \frac{f_{\gamma\gamma}}{f_\gamma} (\gamma')^2, \quad (6)$$

which is a convenient form for numerical solution. Here the function  $f(\gamma)$  is just the right-hand side of (5), subscripts  $\gamma$  indicate derivatives with respect to  $\gamma$ , primes denote derivatives with respect to  $x$ , and  $\nabla_x^2$  is the Laplacian with respect to  $x$ , i.e.,  $\nabla_x^2 \equiv \partial^2 / \partial x^2 + [(d-1)/x] \partial / \partial x$ .

In an earlier treatment of Eqs. (4) and (5), an approximate solution was obtained by expanding  $\gamma dC/d\gamma$  in powers of  $C$  and truncating at  $O(C^3)$  [23]. The Porod tail in the structure factor is lost in this approximation. Despite this, the resulting real-space correlation function was in good agreement with the data of Siegert and Rao [7], although this agreement may be misleading as the data in [7] were not hardened. The present treatment is superior, as no approximations are made beyond the initial gaussian closure. In particular, the Porod tail is present in the solution, as is evident from Figs. 1(b) and 2(b).

The left-hand side of (6) can be written in integral form using the identity [13, 14]

$$\nabla_x^{-2} F(x) = -\frac{1}{d-2} \left[ \int_0^x dy y F(y) \left\{ \left( \frac{y}{x} \right)^{d-2} - 1 \right\} + \int_0^\infty dy y F(y) \right], \quad (7)$$

for  $d > 2$ . (For  $d = 2$  the appropriate limit has to taken [14]). In the context of Eq. (6),  $F(x) = f_\gamma x \gamma'(x) \equiv x f'(x)$  in (7).

To solve Eq. (6) numerically requires specifying boundary conditions at  $x = 0$ . In this paper we specialize to the case  $n = 2$ . Solutions for other values of  $n$  are planned to be presented elsewhere [22]. For  $n = 2$  one can show that  $\gamma(x)$  has a small- $x$  expansion of the form

$$\gamma(x) = 1 - \frac{1}{2} a^2 x^2 - \frac{b x^2}{\ln x} + \dots \quad (8)$$

Therefore the required boundary conditions are  $\gamma(0) = 1$  and  $\gamma'(0) = 0$ . To perform the numerical integration, however, one needs the values of the parameter  $\alpha$  in (6) and the infinite integral  $\int_0^\infty dy y F(y)$  in (7).

Using  $F(x) = xf'(x)$ , this integral can be written as  $-2 \int_0^\infty dy y f(y)$ , which can be expressed in terms of  $\alpha$  and the parameters  $a$  and  $b$  in the small- $x$  expansion (8). Inserting (8) into (6), using (7) to simplify the left-hand side, and matching terms of  $O(1)$  and  $O(1/\ln x)$  gives the relations

$$\alpha = da^2, \quad (9)$$

$$2 \int_0^\infty dy y f(y) = (d-2)(a^2 + 2bd). \quad (10)$$

(Again, the case  $d = 2$  has to be treated separately [14, 22].) Numerical integration of the differential equation (6) is now straightforward, as the finite integral in (7) can be accumulated as the integration proceeds. The two unknown parameters  $a$  and  $b$  are fixed by the requirement that the large- $x$  behavior be physical, i.e.,  $f(x)$  must vanish as  $x \rightarrow \infty$ . For  $d = 3$ , these parameters take the approximate values  $a = 1.177567$  and  $b = -0.155217$ . (For  $d = 2$ , there are still two parameters, but they enter in a slightly different way [22].)

The numerical solutions for the structure factor (the Fourier transform of the pair correlation function) are included in Figs. 1 and 2 as solid lines. Notice that there are no adjustable parameters in the fit. The fit is surprisingly good for  $d = 3$ , despite the fact that the growth law  $L \sim t^{1/4}$  obtained within the Gaussian closure scheme does not have the logarithmic correction predicted for the exact solution. For  $d = 2$ , the fit is noticeably worse. One feature of the approximate theory that is qualitatively incorrect is the small- $k$  behavior. The log-log plots

of Figs. 2(b) and 3(b) show the expected  $k^4$  behavior at small  $k$ . This feature is missing from the Gaussian closure scheme, which gives a  $k^2$  behavior at small  $k$ . Another point of discrepancy between the Gaussian closure theory and the numerical results is that the theory overestimates the amplitude of the Porod tail though it replicates nicely the qualitative features (i.e., valleys and humps), especially in  $d = 3$ . This feature is better seen in a Porod plot of theory and data and we plan to present such a plot elsewhere.

In summary, our simulation data for the conserved XY model is fully consistent, for both  $d = 2$  and  $d = 3$ , with theoretical predictions derived from a scaling assumption [3]. The scaling collapse of the data, using a length scale  $\langle k \rangle^{-1}$  extracted from the structure factor data itself, is good. In future work it would be desirable to test scaling using a length scale derived independently from, for example, the density of vortices (or vortex lines) [5]. An approximate calculation of the structure factor scaling function, using a Gaussian closure scheme, describes the data quite well for  $d = 3$ , except at small  $k$ . We expect this procedure to work even better for  $n > 2$ , where the growth law  $L \sim t^{1/4}$  has no logarithmic corrections [3].

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