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Stress-free spatial anisotropy in phase ordering

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We predict late-time spatial anisotropy for scalar systems with anisotropic surface tension undergoing dissipative quenches below their critical temperature. Spatial anisotropy is confirmed numerically for two-dimensional Ising models with critical and off-critical quenches and with both conserved and nonconserved dynamics. Due to the nonzero anisotropy, expected in all lattice systems, correlation functions in the scaling limit depend on temperature, microscopic interactions, dynamics, disorder, and frustration. [S1063-651X(96)50309-0]

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Most theoretical, numerical, and experimental treatments of nonequilibrium phase-ordering kinetics assume that asymptotic correlations are spatially isotropic in stress-free systems quenched from disordered initial conditions into the ordered phase [1,2]. Numerical measurements in simple Ising models have supported this assumption [3,4], despite several qualitative reports to the contrary [5,6]. It has not been clear whether Potts models [7] and frustrated Ising models [4], where anisotropy effects have been measured, are typical or are special cases. Indeed, without a demonstration that anisotropy is *expected* asymptotically it has been possible to discount measured anisotropy as being a transient effect (see, e.g., [8]).

It is reasonable but not obvious to expect anisotropic *correlations* in phase ordering. The two-dimensional (2D) Ising model below T_c, for example, is spatially anisotropic at arbitrarily large scales in equilibrium correlations [9], in the resulting surface tension [10], and hence in the interface dynamics [11]. In fact, we demonstrate below that spatial anisotropy is *generic* in scalar systems for quenches into an ordered phase with an anisotropic surface tension.

This asymptotic anisotropy leads to many universality classes of phase-ordering correlations, each parametrized by

the functional angle dependence of the effective surface tension as well as, for nonconserved dynamics, by details of the dynamics.

For definiteness, we consider a coarse-grained scalar order parameter, ϕ, in the continuum limit, and define an effective free energy in momentum space $F[\{\phi\}]=\int d^d k[(k^2+D_{\mathbf{k}})\phi_{\mathbf{k}}\phi_{-\mathbf{k}}+V_k]$, where $V_k[\{\phi\}]$ is the Fourier transform of local potential terms and $D_{\mathbf{k}}$ includes anisotropic higher-order gradients. We define an angle dependent free-energy density $\epsilon(\mathbf{n})$ by restricting the integral in F to momenta in a given direction $\mathbf{n}$ and averaging (denoted by angle brackets) over the random initial conditions. To do the restricted momentum integral in $\langle F\rangle$, at late enough times for domain walls to be well defined, we use the anisotropic Porod law for the structure factor $S(\mathbf{k})=\langle\phi_{\mathbf{k}}\phi_{-\mathbf{k}}\rangle$ in general dimension d (generalizing [12]):

$$S(\mathbf{k})\simeq 2^{d+2}\pi^{d-1}A k^{-(d+1)}P(\mathbf{k}/k), \tag{1}$$

which holds for $L^{-1}\ll|\mathbf{k}|\ll\xi(\mathbf{n})^{-1}$, where $L(t)$ is the characteristic growing length scale of the system and $\xi(\mathbf{n})$ is the domain wall width for domain walls with normal orientation $\mathbf{n}=\mathbf{k}/k$. $A(t)\sim L^{-1}$ is the average area density of domain wall and $P(\mathbf{n})$ is the angle distribution function of domain wall orientation. We find

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$$\epsilon(\mathbf{n}) = A\sigma(\mathbf{n})P(\mathbf{n}), \qquad (2)$$

where the leading k^2 and potential terms make isotropic contributions to $\sigma(\mathbf{n})$, while $D_{\mathbf{k}}$ makes anisotropic contributions both directly and through $\xi(\mathbf{n})^{-1}$. From Eq. (2) we identify $\sigma(\mathbf{n})$ as the effective angle dependent surface tension for domain walls with normal direction $\mathbf{n}$ [13].

Now consider a dissipative quench to $T = 0$, with no thermal noise. The dynamics will be given by $\dot{\phi}_{\mathbf{k}} = -\Gamma(\mathbf{k})\delta F/\delta\phi_{-\mathbf{k}}$, where the dot indicates a time derivative. We assume leading behavior of $\Gamma = \mathrm{const}$, which corresponds to nonconserved dynamics, or $\Gamma = \Gamma_2 k^2$, which corresponds to conserved dynamics [14]. The time rate of change of the energy density is then simply [15]

$$\dot{\epsilon}(\mathbf{n}) = \int dk \, k^{d-1} \langle \delta F/\delta\phi_{\mathbf{k}} \dot{\phi}_{\mathbf{k}} \rangle$$

$$= -\int dk \, k^{d-1} \Gamma^{-1} \langle \dot{\phi}_{\mathbf{k}} \dot{\phi}_{-\mathbf{k}} \rangle, \qquad (3)$$

where $\mathbf{k} \equiv k\mathbf{n}$. We have used the dynamics of ϕ to replace the functional derivative of the free energy so that the resulting expression for $\dot{\epsilon}(\mathbf{n})$ has no *explicit* dependence on $F[\{\phi\}]$ or, hence, on $\sigma(\mathbf{n})$.

Imposing isotropic correlations generally leads to a contradiction *if the surface tension is anisotropic* — different anisotropies in Eqs. (2) and (3). This implies that *the correlations are anisotropic at arbitrarily late times.*

It is easy to see that anisotropic correlations are needed to have consistency between the two expressions for the energy density. Apart from anisotropic correlations, the anisotropy of $\epsilon(\mathbf{n})$ in Eq. (2) is determined by the statics, through $\sigma(\mathbf{n})$. On the other hand, the anisotropy of $\dot{\epsilon}(\mathbf{n})$ in Eq. (3) is determined by the dynamics, through $\Gamma(\mathbf{k})$, in addition to possible contributions by the effective UV cutoff $\xi(\mathbf{n})^{-1}$. Since σ and Γ are independent, the anisotropies of Eqs. (2) and (3) will not generally be equal unless anisotropic correlations make up the difference. For more general forms of the free energy $F[\{\phi\}]$ and dynamics $\Gamma(\mathbf{k})$ the *same argument applies*, as long as the energy density is represented by Eqs. (2) and (3).

The renormalization-group (RG) approach to phase ordering [16] is easily generalized to include anisotropy. The only change is to note that any anisotropy of either $F[\{\phi\}]$ or $\Gamma(\mathbf{k})$ will be renormalized by microscopic details. (An illustration of this renormalization is the temperature dependence of the effective surface tension [10].) The demonstration that thermal noise will be asymptotically irrelevant for quenches below T_c will still apply, with the caveat that the effective $T = 0$ dynamics will include the effective surface tension at the quench temperature. We then apply our above argument that predicts anisotropy with noise free dynamics. As a result, we expect anisotropy for all scalar quenches below T_c [17].

The surface tension will depend on temperature, disorder, and the details of the local interactions in the system, but will be independent of the dynamics at late times. Since the surface tension always enters into Eq. (2), it will affect anisotropic correlations in the scaling limit.

What about the dynamics? The RG approach [16] shows that $\Gamma(\mathbf{k})$ will only be renormalized analytically, i.e., anisotropy will only enter at $O(k^4)$ and higher. For conserved dynamics, where $\Gamma(\mathbf{k}) = k^2$ to leading order [14], anisotropic contributions are subdominant in Eq. (3) since the integral converges in the UV [15]. Thus neither the anisotropy of $\Gamma(\mathbf{k})$ nor the anisotropy of the core scale $\xi(\mathbf{n})$ will affect $\dot{\epsilon}(\mathbf{n})$ through Eq. (3). For conserved dynamics then, the anisotropy of the surface tension alone (an equilibrium property) determines the anisotropy of the correlations.

With nonconserved dynamics, where $\Gamma = \mathrm{const}$ to leading order, the UV regime dominates the energy-dissipation integral (3) [15] and both $\Gamma(\mathbf{k})$ and $\xi(\mathbf{n})$ make anisotropic contributions to $\dot{\epsilon}(\mathbf{n})$. As a result, anisotropy will in general depend on the details of the microscopic dynamics, even including global conservation laws that are "irrelevant" [16] in terms of growth laws. In principle the anisotropy of $\Gamma(\mathbf{k})$ could then be renormalized to compensate $\sigma(\mathbf{n})$; in practice we numerically find anisotropy in all cases.

For the remainder of this paper, we explore 2D Ising models with nearest-neighbor interactions on a periodic square lattice under quenches from random initial conditions. For a system defined on a lattice, anisotropies will be present in the surface tension below T_c, because lattice interactions are not rotationally invariant. Our argument then implies anisotropic correlations in the scaling limit. Indeed, we find anisotropic correlations quite generally — for a variety of temperatures below T_c, of initial magnetizations, and for all of globally conserved, nonconserved, and locally conserved dynamics. These anisotropies do not decrease at late times, as would be expected for transient effects introduced by the dynamics at earlier times.

We measure the normalized correlations $C(\mathbf{r}, t) = [\langle \phi(\mathbf{r})\phi(0)\rangle - \langle\phi\rangle^2]/[\langle\phi(0^+)\phi(0)\rangle - \langle\phi\rangle^2]$, which ranges from 1 at short distances to 0 at infinity [13]. The anisotropic length scale $L(\mathbf{n}, t)$ of a system is defined by the scale in direction $\mathbf{n}$ at which $C = 0.5$ for nonconserved dynamics, and by the first zero of C for conserved dynamics. We scale correlations in all directions by the length scale in the diagonal direction. A natural measure of anisotropy is $\chi = (L_{max}/L_{min} - 1)/(\sqrt{2} - 1)$, where L_{max} is the maximum length scale at a given time and L_{min} is the minimum, and so χ runs from 0 (circle) to 1 (square) for convex contours of $C(\mathbf{r})$.

We first consider off-critical quenches with a global conservation law to prevent the magnetization from saturating. We couple the system to a Creutz spin reservoir of size 2 [18]: each randomly chosen spin is updated by a Metropolis algorithm, subject to an additional microcanonical constraint that any spin change (± 2) fits in the spin reservoir. We study size 1024^2 systems with $\langle\phi\rangle = 0.4$. A snapshot from a quench to $T = 0.2T_c$ in Fig. 1 illustrates the strong anisotropy even above the roughening transition [19]. We show some contour plots of the scaled correlations in Fig. 2. It is clear that the anisotropies are not limited to the small r regime. The anisotropy is increasing at late times (see inset of Fig. 3). In the same regime, the spherically averaged correlations scale well. The latest anisotropies, at $t = 2049$ Monte Carlo steps (MCS's), before finite-size effects entered were
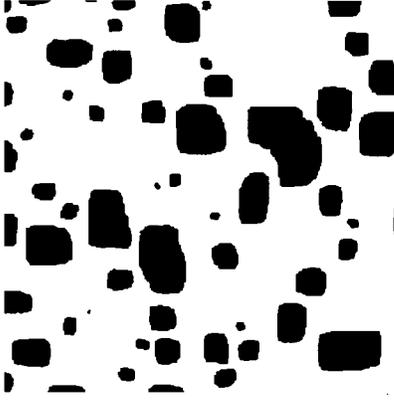
FIG. 1. A 512^2 region of a globally conserved $T/T_c = 0.2$ quench with $\langle \phi \rangle = 0.4$ ($t = 513$ MCS's). Lattice directions, here and in the next figure, are vertical and horizontal.

$\chi = 0.45$ ($T = 0$), 0.38 ($T = 0.2T_c$), and 0.12 ($T = 0.4T_c$). (Statistical error bars, with at least 30 samples in each case, are less than ± 0.001.)

We also studied nonconserved critical quenches. With heat-bath dynamics and a sublattice update, late times in large lattices could be reached. Even so, the asymmetry remained small. For lattices of size 2048^2, and a quench to $T = 0$, we show dC/dx vs x ($x = r/L$), along the diagonal and lattice directions, in Fig. 3. We find $\chi = 0.03$ at the latest time ($t = 4097$ MCS's, 74 samples, statistical error ± 0.0003). The constant but orientation dependent domain wall width, $\xi(\mathbf{n})$, evident in the sharp downturn of dC/dx near $x = 0$ in the diagonal correlations, increases χ by $O(1/L)$. This is significant for small anisotropies and early times [20]. Directly subtracting this $O(1/L)$ contribution
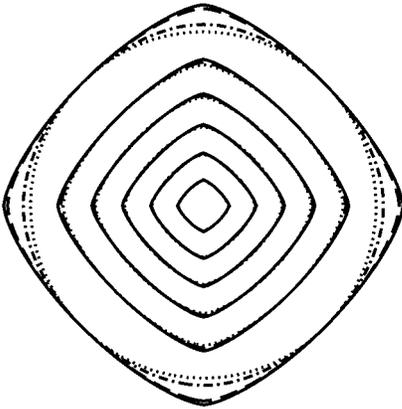
FIG. 2. Anisotropic contours of scaled correlations $C(\mathbf{r}/L) = 0.9$, 0.8, 0.7, 0.6, and 0.5 (from the center) for an off-critical quench to $T = 0$ with $\langle \phi \rangle = 0.4$ and globally conserved Creutz dynamics. The times are $t = 513$ MCS's (dotted), 1025 (dashed), and 2049 (solid). Also shown, scaled by 1.4 for clarity, are the $C = 0.5$ contours of quenches to $T/T_c = 0$, 0.2, 0.4, and 0.9 (solid, dashed, dot-dashed, and dotted lines, respectively) at $t = 1025$ MCS's. The length scale L is such that, along the diagonal direction, $C(L) = 0.5$. Circular (square) contours correspond to $\chi = 0$ (1).
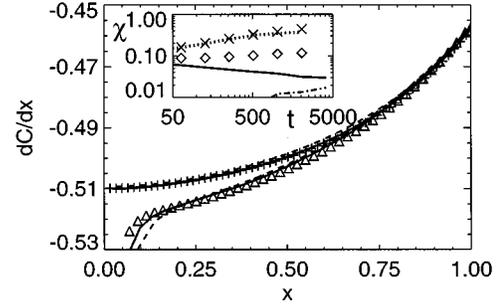
FIG. 3. dC/dx vs scaled distances, x, for a nonconserved critical quench to $T = 0$. The plusses indicate correlations in the lattice axis direction, while the triangles indicate correlations along lattice diagonals (at $t = 4097$ MCS's). Solid and dashed lines indicate corresponding correlations at $t = 2049$ and 1025 MCS's, respectively. In the inset is the anisotropy measure χ vs t for $T/T_c = 0$, 0.2, and 0.4 globally conserved quenches from Fig. 2 (crosses, dotted lines, and diamonds, respectively). At the bottom of the inset are the bare and corrected χ (solid and dot-dashed lines, respectively) for the nonconserved quench of the main figure.

leads to χ slowly increasing with time (inset of Fig. 3), with a corrected latest value $\chi = 0.02$.

We have also simulated conserved 2D Ising systems with nearest-neighbor Kawasaki exchange dynamics and a Metropolis update. At low enough temperatures for the anisotropy of $\sigma(\mathbf{n})$ to be visible, the activated dynamics slows the simulations considerably. We explored size 256^2 systems, with $\langle \phi \rangle = 0.4$ and $T = 0.4T_c$, up to times $t = 10^6$ MCS's (10 samples). The length scales achieved ($L \lesssim 12$) are so small that $\chi \approx 0$ within numerical accuracy, so in Fig. 4 we plot $C(\mathbf{r})$ against the energy-energy correlation function $C_E(\mathbf{r}) \equiv \langle E(\mathbf{r})E(0) \rangle / \langle E \rangle^2 - 1$, where $E(\mathbf{r})$ is the number of broken bonds at site $\mathbf{r}$ minus the equilibrium bulk average. This shows a significant and increasing difference between correlations in the lattice and diagonal directions.

In summary of our numerical results, we find anisotropic correlations in various quenched 2D Ising models. Anisotropy increases with decreasing temperature and for increasing net magnetization. Anisotropy effects are always slowly
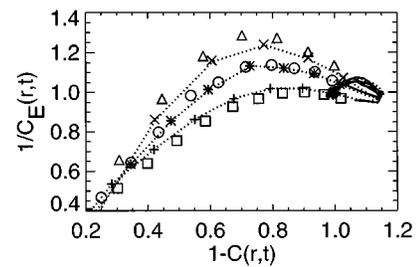
FIG. 4. Two-point correlations vs energy-density correlations for a conserved quench to $T/T_c = 0.4$ with $\langle \phi \rangle = 0.4$ (size 256^2). The correlations are spherically averaged (stars and circles), along the axis (plusses and squares), and along the diagonal (crosses and triangles). For clarity, solid lines have been used after the first zero of C. Times are 2.6×10^5 and 1.0×10^6 MCS's, respectively. Dotted lines show data from size 128^2 systems (36 samples) at the earlier time.

increasing at the latest times of our simulations. In all of our simulations, the spherically averaged correlations scale reasonably well while the anisotropy is still evolving. To study the nonzero asymptotic anisotropy in these systems, some sort of acceleration method is needed (see, e.g., [6]) — though with nonconserved dynamics the anisotropy will depend on the numerical algorithm used.

In disordered [1,21] and frustrated [4,8] models, it has been argued that scaling functions will be ''universal'' — identical to simple Ising models. While logarithmic growth is seen, it is thought to come from effective L dependence in the kinetic prefactor Γ — so that scaled correlations are unaffected. If this picture is correct, and scaling function universality holds in these systems (in the broad sense described in the introduction), then the results of this paper directly apply and anisotropy will be present in disordered or frustrated lattice systems [22]. Indeed, in frustrated Ising models, fairly large anisotropy is seen numerically [4,8]. Hopefully, in experimental random-field systems (e.g., [23]), anisotropy can be tested directly.

We can generalize our argument around Eqs. (1)–(3) to systems with other types of singular defects. Using vector $O(n)$ order parameters, and a generalized Porod's law $S(\mathbf{k}) = D(\mathbf{k}/k)L^{-n}k^{-(d+n)}$ [1], we find that the anisotropic contribution to the energy density is asymptotically negligible for systems without domain walls [24]. However, other systems with dissipative dynamics in which domain walls dominate the asymptotic energetics will be anisotropic if the surface tension is anisotropic, e.g., Potts models (see [7]).

The growth laws of the characteristic length scale $L(t)$ will remain independent of any anisotropies present, as long as dynamical scaling is maintained. This follows from the energy-scaling approach [15] since anisotropy does not change the scaling properties of the energy or the rate of energy dissipation. We would be surprised if the anisotropy affected the dynamical scaling of the correlations (see, however, [6]), though the scaling regime seems to be pushed to much later times as the anisotropy slowly develops. (In addition, scaling functions will in general be functions of orientation as well as scaled distance, as is discernible in Figs. 3 and 4.) It remains an open question whether nonzero anisotropies have implications beyond the scaled correlations, such as in autocorrelation exponents.

In practice, isotropic theories have worked fairly well for spherically averaged correlations. Certainly, lattices, interactions, and dynamics can be chosen to minimize anisotropies. This would be desirable, for instance, in lattice simulations of isotropic fluid or polymer systems. However, the language of an *isotropic* zero-temperature phase-ordering fixed point is inappropriate for a scalar system with an anisotropic surface tension.

In summary, we expect anisotropy for any scalar lattice system quenched to below T_c, including disordered and-or frustrated systems. The anisotropy will depend on the details of the system.

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