Kinetics of ordering for correlated initial conditions

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Nonequilibrium domain growth in a system with a nonconserved order parameter is considered for power-law correlated initial conditions, $[\phi(\mathbf{r})\phi(\mathbf{0})] \sim r^{-(d-\sigma)}$, appropriate to, e.g., a quench to the ordered phase from the critical point ($\sigma=2-\eta$). The long-range correlations are shown to be *relevant* (in the renormalization-group sense), and lead to a new scaling function for the structure factor, provided that σ exceeds a critical value. In this regime (which includes $\sigma=2-\eta$) the autocorrelation function $A(t)\equiv[\phi(\mathbf{r},t)\phi(\mathbf{r},0)]$ has the asymptotic behavior $A(t)\sim t^{-(d-\sigma)/4}$.

The kinetics of domain growth following the quench of a system from the disordered to the ordered phase has generated a vast literature.[1] For a conserved order parameter this is the phenomenon of phase separation or "spinodal decomposition." Here we will be interested in the case of a nonconserved order parameter, appropriate for the order-disorder transitions observed in many binary alloy systems. We will show that when the initial conditions exhibit power-law spatial correlations of sufficiently long range, a new universality class is obtained, with a time-dependent structure factor and temporal correlation functions which depend explicitly on the exponent characterizing the correlations in the initial conditions. A special case of experimental relevance is when the initial condition is the equilibrium critical state. The present study complements the recent investigations of scaling behavior following a quench from the high-temperature phase *to* the critical point,[2] and completes the "triangle" of possible quenches (high-to-low, high-to-critical, critical-to-low).

A central quantity in the study of domain growth is the time-dependent structure factor $S_{\mathbf{k}}(t)=[\phi_{\mathbf{k}}(t)\phi_{-\mathbf{k}}(t)]$, where $\phi_{\mathbf{k}}$ is a Fourier component of the (scalar) order parameter and square brackets indicate an average over initial conditions. For simplicity we will work at $T=0$, since thermal fluctuations should be asymptotically irrelevant for a quench into the ordered phase. The structure factor is expected to having the scaling form[1]

$$S_{\mathbf{k}}(t)=L(t)^d g_e(kL(t)) , \tag{1}$$

where d is the dimensionality of space and the domain scale $L(t)\sim t^{1/2}$ for a nonconserved order parameter.[3] Recently we have introduced[4] a second fundamental quantity, the response to the initial condition, defined by $G_{\mathbf{k}}(t)=[\partial\phi_{\mathbf{k}}(t)/\partial\phi_{\mathbf{k}}(0)]$. It has the scaling form

$$G_{\mathbf{k}}(t)=L(t)^{\lambda} g(kL(t)) , \tag{2}$$

where λ is a new nontrivial exponent and $g(0)=\text{const}$. The scaling forms (1) and (2) apply when t is large compared to microscopic time scales: by definition, $G_{\mathbf{k}}(0)=1$. For initial conditions with only short-range correlations, λ has been calculated to first order in $1/n$ for an n-component vector order parameter.[4]

If the initial conditions are Gaussian random variables with correlation function $[\phi_{\mathbf{k}}(0)\phi_{-\mathbf{k}'}(0)]=\delta_{\mathbf{k},\mathbf{k}'}\Delta(k)$, integration by parts relates $G_{\mathbf{k}}(t)$ to the correlator $C_{\mathbf{k}}(t)$ of the field with the initial condition:

$$C_{\mathbf{k}}(t)\equiv[\phi_{\mathbf{k}}(t)\phi_{-\mathbf{k}}(0)]=\Delta(k)G_{\mathbf{k}}(t) . \tag{3}$$

Although (3) is strictly true only for Gaussian initial conditions, we conjecture that it holds more generally in the scaling regime, i.e., that higher cumulants of the initial condition distribution are irrelevant in the renormalization-group (RG) sense. This can readily be confirmed for a vector order parameter with $n=\infty$, where only the second cumulant of the distribution enters, and in the $d=1$ Glauber model (see below). A scaling form for the more general correlation function $[\phi_{\mathbf{k}}(t)\phi_{-\mathbf{k}}(t')]$, with t and t' both large, can also be written down,[4,5] but involves no additional exponents.

The dependence of the ordering kinetics on the nature of the initial conditions has not been adequately addressed in previous work. In this Brief Report we consider the case where $\Delta(k)$ contains a component corresponding to long-range (power-law) correlations, i.e.,

$$\Delta(k)=\Delta_{\mathrm{SR}}+\Delta_{\mathrm{LR}}k^{-\sigma} , \tag{4}$$

with $0<\sigma<d$. Then the correlations in real space decay as $r^{-(d-\sigma)}$. Using elementary renormalization-group arguments, we predict that the exponent λ defined by (2) retains its short-range value λ_{SR} for $\sigma<\sigma_c=d-2\lambda_{\mathrm{SR}}$, while $\lambda=(d-\sigma)/2$ exactly for $\sigma>\sigma_c$. More generally, the long-range correlations are irrelevant (relevant) for $\sigma<\sigma_c$ ($\sigma>\sigma_c$). In consequence, the scaling function for the structure factor retains its short-range form for $\sigma<\sigma_c$, but acquires a new, σ-dependent form for $\sigma>\sigma_c$. In particular, for a small scaling variable $k^2t\to 0$, we predict $S_{\mathbf{k}}(t)\sim k^{-\sigma}t^{(d-\sigma)/2}$ for $\sigma>\sigma_c$. These conclusions are supported by the $1/n$ expansion for a vector order parameter, by exact results for the $d=1$ Ising model with Glauber dynamics, and by Monte Carlo simulations of the $d=2$ Ising model.

The RG calculation follows a familiar path, albeit in the context of the $T=0$ fixed point that controls domain growth. Note, however, that we do not explicitly demonstrate, by deriving recursion relations, the existence of a

RG fixed point from which the scaling forms (1) and (2) emerge. Rather, scaling is assumed and the existence of an underlying RG inferred. The scaling hypothesis is, however, supported by a wealth of experimental and simulational evidence,[1] and the scaling forms (1) and (2) can be derived explicitly for a vector order parameter within a $1/n$ expansion[4] and for the $d=1$ Ising model with Glauber dynamics.[6] On the other hand, the large-n limit for a *conserved* vector order parameter reveals a more complicated scaling form than (1), involving two marginally different length scales.[7] Subject to the above caveats, a schematic RG calculation may be performed as follows. Starting from the deterministic Langevin equation $d\phi_{\mathbf{k}}/dt=-\partial H/\partial\phi_{\mathbf{k}}$, where H is the Hamiltonian, one formally eliminates Fourier components with $\Lambda/b<|\mathbf{k}|<\Lambda$, with Λ the large-momentum cutoff and b the RG scale parameter. Then one rescales momenta, times, and fields according to $\mathbf{k}=\mathbf{k}'/b$, $t=b^2t'$, $\phi_{\mathbf{k}'/b}(b^2t')=b^{\zeta}\phi'_{\mathbf{k}'}(t')$, and $\phi_{\mathbf{k}'/b}(0)=b^{\chi}\phi'_{\mathbf{k}'}(0)$. Note the introduction of a separate scaling dimension for the initial condition. Applying these rescalings to the scaling forms (1) and (2) determines the exponents ζ and χ: $\zeta=d/2$ and $\chi=d/2-\lambda$.

Under the RG transformation the correlator $\Delta(k)$ of the initial condition, defined through $[\phi_{\mathbf{k}}(0)\phi_{-\mathbf{k}}(0)]=\Delta(k)$, becomes $b^{2\chi}[\phi'_{\mathbf{k}'}(0)\phi'_{-\mathbf{k}'}(0)]=\Delta(k'/b)+\cdots$, where the ellipsis indicates the contribution from the coarse-graining stage of the RG. Thus the new initial correlator $\Delta'(k')=[\phi'_{\mathbf{k}'}(0)\phi'_{-\mathbf{k}'}(0)]$ is given by

$$\Delta'(k')=b^{2\lambda-d}\{\Delta(k'/b)+\cdots\}\ . \tag{5}$$

Using (4) we can write flow equations for the short- and long-range parts of the correlator:

$$\Delta'_{\mathrm{SR}}=b^{2\lambda-d}\{\Delta_{\mathrm{SR}}+\cdots\}\ , \tag{6}$$

$$\Delta'_{\mathrm{LR}}=b^{2\lambda-d+\sigma}\Delta_{\mathrm{LR}}\ . \tag{7}$$

The key point here is the absence of any contribution to Δ'_{LR} from the elimination of short length scales. This kind of result is familiar from the study of critical phenomena in systems with long-range interactions,[8,9] long-range correlated disorder,[10] or long-range correlated random fields,[11] etc., and a similar result for the renormalization of the transport coefficient was recently used to derive the $t^{1/3}$ domain growth law for a *conserved* scale order parameter.[12] The common feature of these calculations is the absence of any additional singularities at small momenta arising from the elimination of large momenta.

At the fixed point controlling domain growth, both the equation of motion and the initial condition distribution should be invariant under the RG transformation. It follows immediately from (7) that the long-range correlations are irrelevant (i.e., Δ_{LR} iterates to zero) at the "short-range fixed point" if $\sigma<d-2\lambda_{\mathrm{SR}}$. In the opposite regime, the invariance of Δ_{LR} at the "long-range fixed point" fixes $\lambda_{\mathrm{LR}}=(d-\sigma)/2$. The determination of λ_{SR} is nontrivial, since it requires explicit computation of the terms represented by the ellipsis in (6). To first order in $1/n$, where n is the internal dimension of a vector order parameter, one finds[4] $\lambda_{\mathrm{SR}}=d/2-a(d)/n$, where $a(d)$ (>0) is given in Ref. 4, so $\sigma_c=2a(d)/n+O(1/n^2)$. The validity of Eq. (7) is also confirmed by the $1/n$ expansion,[13] since one finds no correction to $\lambda_{\mathrm{LR}}=(d-\sigma)/2$. Note that a naive interpretation of the $1/n$ results would predict that λ is discontinuous at $\sigma=0$. Here, as elsewhere,[9-11] one needs the RG to interpret the results correctly.

Consider now the functions $S_{\mathbf{k}}(t)$, $G_{\mathbf{k}}(t)$, and $C_{\mathbf{k}}(t)$ of Eqs. (1)–(3). The scaling functions $g_e(x)$ and $g(x)$ will have the short-range forms for $\sigma<\sigma_c$, but will depend on σ for $\sigma>\sigma_c$. Note, however, that because of the explicit factor of $\Delta(k)$ in (3), $C_{\mathbf{k}}(t)$ picks up the $k^{-\sigma}$ term from (4), which dominates over the constant term in the scaling limit $k\to 0$. Thus $C_{\mathbf{k}}(t)=\Delta_{\mathrm{LR}}k^{-\sigma}t^{\lambda/2}\tilde{g}(k^2t)$. Summing over $\mathbf{k}$ yields the autocorrelation function $A(t)\equiv[\phi(\mathbf{r},t)\phi(\mathbf{r},0)]\sim t^{-(d-\sigma-\lambda)/2}$. In the long-range regime, this becomes $A(t)\sim t^{-(d-\sigma)/4}$. The two forms match, as expected, at $\sigma=\sigma_c$. When the initial state is the critical state, $A(t)\sim t^{-(d-2+\eta)/4}$. For the $d=2$ Ising model ($\eta=\frac{1}{4}$), for example, we predict $A(t)\sim t^{-1/16}$.

The structure factor $S_{\mathbf{k}}(t)$ also has, even for $\sigma<\sigma_c$, a "long-range" contribution $S_{\mathbf{k}}^{\mathrm{LR}}(t)$ varying as $k^{-\sigma}$ at small k. It is given by the diagram of Fig. 1, where the circle represents $\Delta(k)$ and the lines are exact response functions. Thus $S_{\mathbf{k}}^{\mathrm{LR}}(t)=\Delta_{\mathrm{LR}}k^{-\sigma}G_{\mathbf{k}}(t)G_{-\mathbf{k}}(t)$. The remaining contributions to $S_{\mathbf{k}}(t)$ should be finite at $k=0$. This structure has been confirmed explicitly in the $1/n$ expansion.[13] Using Eq. (2) gives $S_{\mathbf{k}}^{\mathrm{LR}}(t)=k^{-\sigma}t^{\lambda}s(k^2t)$, with $s(0)=\mathrm{const}$. Comparing this with the general scaling form (1), we observe that, for $\lambda+\sigma/2<d/2$ (i.e., for $\sigma<\sigma_c$), $S_{\mathbf{k}}^{\mathrm{LR}}(t)$ *does not contribute to the scaling function,* i.e., it is negligible compared to the full $S_{\mathbf{k}}(t)$ in the scaling limit $k\to 0$, $t\to\infty$ at fixed k^2t. For $\sigma>\sigma_c$, the scaling function *is* long-ranged, i.e., $g_e(x)\sim x^{-\sigma}$ for $x\to 0$ in Eq. (1). In real space, this means that for $\sigma>\sigma_c$ the equal-time correlation function $C(r,t)\equiv[\phi(\mathbf{r},t)\phi(\mathbf{0},t)]$ decays as $\{L(t)/r\}^{d-\sigma}$ for $r\gg L(t)$.

For $d=1$, the Ising model with Glauber dynamics can be solved exactly.[14] For $T=0$ and small k one obtains $\langle\phi_{\mathbf{k}}(t)\rangle=\phi_{\mathbf{k}}(0)\exp(-k^2t)$ for the Fourier components of the Ising spins, where $\langle\ \rangle$ indicates an average over the residual noise present in Glauber dynamics at $T=0$. Incorporating this latter average into [ ], the result $G_{\mathbf{k}}(t)=\exp(-k^2t)$ for the response function follows immediately. Comparison with (2) gives $\lambda=0$, and hence $\sigma_c=1$. Thus long-range correlations are irrelevant (in the RG sense) for all physical values of σ (i.e., $\sigma<d=1$),

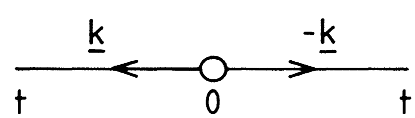

FIG. 1. Diagram for $S_{\mathbf{k}}^{\mathrm{LR}}(t)$. A line and a circle represent the response function (2) and the correlator (4), respectively.

as shown explicitly by Bray.[6] The correlation with the initial condition is $C_{\mathbf{k}}(t)=\Delta(k)\exp(-k^2t)$, so the autocorrelation function is $A(t)\sim t^{-(1-\sigma)/2}$, generalizing the $t^{-1/2}$ dependence found for initial conditions with short-range correlations.[6] We note also that Eq. (3) holds exactly for this model, due to the linear dependence of $\langle\phi_{\mathbf{k}}(t)\rangle$ on $\phi_{\mathbf{k}}(0)$.

The case of greatest experimental relevance is $\sigma=2-\eta$, corresponding to a quench from the equilibrium state at T_c. To determine whether this belongs to the short- or long-range universality class we need to know λ_{SR}. Monte Carlo simulations[15] of the Ising model suggest $\lambda_{SR}\simeq\frac{3}{4}$ and $\frac{3}{2}$ for $d=2$ and 3, respectively, giving $\sigma_c\simeq\frac{1}{2}$ and 0, respectively. Thus σ_c is definitely less than $2-\eta$ ($=\frac{7}{4}$ and $\simeq 2$, respectively) placing these systems firmly in the long-range universality class. This implies a $t^{-(d-2+\eta)/4}$ decay for the autocorrelation function $A(t)$, i.e., $t^{-1/16}$ for $d=2$ and $\simeq t^{-1/4}$ for $d=3$, and a structure factor of the form

$$S_{\mathbf{k}}(t)=k^{-(2-\eta)}t^{(d-2+\eta)/2}s(k^2t)$$

with $s(0)=\text{const}$.

Monte Carlo simulations on the $d=2$ Ising model have been performed to test these predictions. Equilibrium states at $T=T_c=2/\ln(1+\sqrt{2})$ were prepared[16] using the accelerated convergence algorithm of Wolff.[17] Each such state was then quenched to $T=0$ and evolved using conventional "heat-bath" dynamics,[18] vectorized by sequential updating of each sublattice in turn. The equal-time correlation function $C(r,t)=[S_i(t)S_j(t)]$, with sites i and j separated by r lattice spacings along a lattice direction, is presented in scaling form in the inset in Fig. 2, where t is the elapsed time after the quench in units of attempted updates per spin. The data represent an average over 100 independent initial conditions for a system of size 250^2 with periodic boundary conditions. What is actually plotted is $\tilde{C}(r,t)=C_L(r,t)[C_\infty(r,0)/C_L(r,0)]$, where C_L and C_∞ are the correlation functions for the finite and infinite lattices, respectively.[19] This correction is designed to remove, as far as possible, finite-size effects in the spatial correlations at $t=0$, this being the dominant finite-size effect present. Its efficacy is demonstrated by the exceptionally good scaling plot obtained. A further refinement was to select only initial equilibrium states with magnetization per site M satisfying $|M|<0.01$. If all equilibrium states are included, the data fall on the same scaling curve at short times, but break away at later times. This is because finite-size scaling yields $|M|\sim L^{-\beta/\nu}=L^{-1/8}$, so $|M|$ is typically large ($|M|\sim 0.6$ for $L=250$). As a result, the system usually reaches a single domain quite quickly. Selecting initial states with small M is a device to artificially expand the scaling regime. The dashed curve shows the asymptotic behavior $C(r,t)\simeq 0.96\,(\sqrt{t}/r)^{1/4}$, with the same r dependence as the initial condition, as predicted for the long-range universality class. This scaling function is quite different from that associated with the conventional quench from

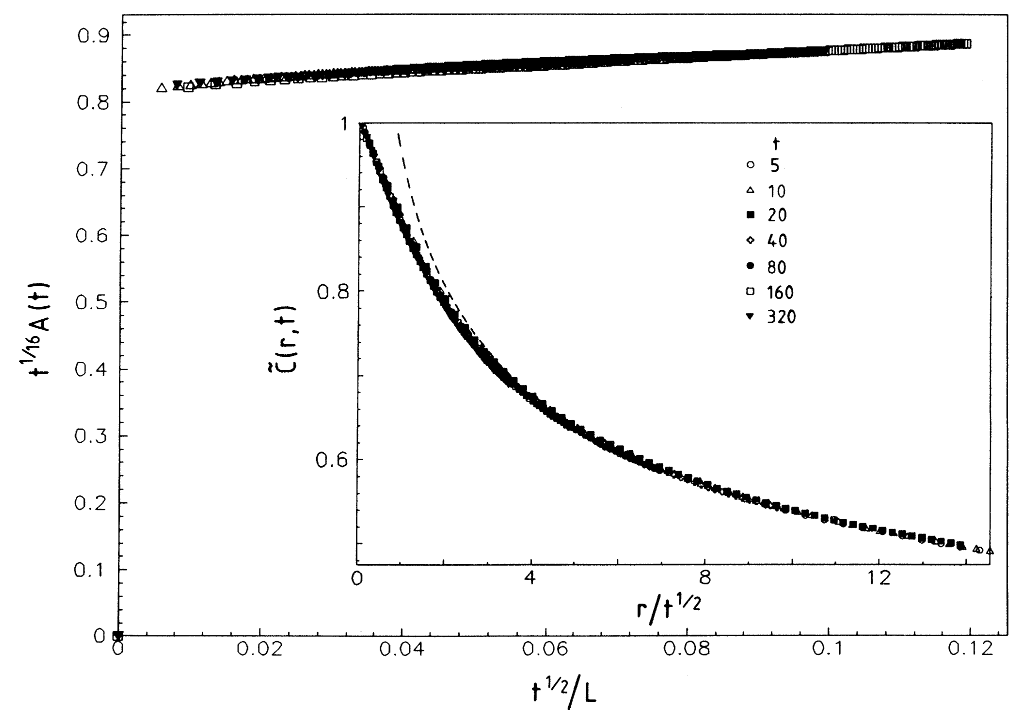

FIG. 2. Finite-size scaling plot for the autocorrelation function of the two-dimensional Ising model quenched from $T=T_c$ to $T=0$. △, $L=250$; ▼, $L=180$; □, $L=150$. Inset: Scaling plot for the equal-time correlation function. The dashed curve is the asymptotic behavior $C(r,t)\simeq 0.96(\sqrt{t}/r)^{1/4}$.

the high-temperature phase.[1]

The results for the autocorrelation function are consistent with the prediction $A(t) \sim t^{-1/16}$. In this case we were unable to correct simply for the finite-size effects on the initial condition, which yield a $C_L(r,0)$ decreasing more slowly than $1/r^{1/4}$. As a result, we expect $A(t)=t^{-1/16}a(\sqrt{t}/L)$, the argument of the scaling function a being the ratio of the domain scale to the system size. Therefore we employ a finite-size scaling analysis, in which a plot of $t^{1/16}A(t)$ versus $\sqrt{t}/L$ should collapse the data. The result is shown in Fig. 2. The data collapse is quite satisfactory.

In summary, a new universality class for domain growth from correlated initial conditions has been identified. The nontrivial exponent λ that enters the scaling form for the response function has been determined exactly for this class. The scaling function for the structure factor has a new universal form characterized by the range of the correlations in the initial conditions. The results are relevant to a quench into the ordered phase from the critical point.

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