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Domain coarsening in two dimensions: Conserved dynamics and finite-size scaling

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We present results from a study of finite-size effect in the kinetics of domain growth with conserved order parameter for a critical quench. Our observation of a weak size effect is a significant and surprising result. For diffusive dynamics, appropriate scaling analysis of Monte Carlo results obtained for small systems using a two-dimensional Ising model also shows that the correction to the expected Lifshitz-Slyozov law for the domain growth is very small. The methods used in this work to understand the growth dynamics should find application in other nonequilibrium systems with increasing length scales.

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The kinetics of phase separation in a binary mixture, A_1+A_2, when quenched below the coexistence curve is an active research area [1]. The growth of domains, rich in A_1 or A_2 particles, during the phase separation is a scaling phenomenon, e.g., the two-point equal-time (t) correlation function, $C(r,t)$, characterizing the domain morphology and growth, exhibits the scaling form [2]

$$C(r,t) \equiv \widetilde{C}(r/\ell(t)), \tag{1}$$

where $\widetilde{C}(x)$ is a scaling function independent of the average domain linear dimension $\ell(t)$, which grows as $\ell(t) \sim t^{\alpha}$.

While recent focus has been on systems with realistic interactions and other physical conditions [3], often the growth exponent α is poorly understood even in simple systems due to the lack of appropriate method of analyzing simulation results. Most of the simulation studies, to date, have stressed the value of using large systems, with the anticipation of strong finite-size effects combined with the expectation that the predicted growth laws will be realized only for $\ell(t\to\infty)\to\infty$, while also leading to better self-averaging. Typical system sizes authors consider these days contain numbers of lattice sites or particles of the order of a million, which is too large, even for present day computers, to access long time scales that are often necessary.

The primary objective of this Rapid Communication is to study finite-size effects in domain coarsening with diffusive dynamics following a *critical quench*. We chose to employ, as a prototype for a large class of phase transition with critical points, a $(d=2)$-dimensional Ising model with Hamiltonian

$$H = -J\sum_{\langle ij\rangle} S_i S_j, \quad S_i = \pm 1, \quad J > 0. \tag{2}$$

In particular we wish to understand the behavior of the effective or instantaneous exponent α as a function of time. For a conserved order parameter with diffusive dynamics, associating the rate of domain growth with the gradient of chemical potential, one can write [1]

$$d\ell(t)/dt \sim |\vec{\nabla}\mu| \sim \sigma/\ell(t)^2, \tag{3}$$

where σ is the A_1-A_2 interfacial tension. Solving Eq. (3) one gets $\alpha=1/3$, known as the Lifshitz-Slyozov (LS) [4] growth law. However for fluid systems where hydrodynamics is important one expects faster growth [1].

We show here via the application of finite-size scaling methods [5] that the LS value of α is realized very early after the initial quench. This contradicts earlier [6] understandings. Furthermore, effect of size is rather small so that using a system as small as $L^2=16^2$, one can confirm the LS growth law unambiguously. Even though this study is based on the conserved Ising kinetics in $d=2$, we expect our observation, understanding, and technique to find relevance in other systems exhibiting growing length scales, e.g., ordering in ferromagnets, surface growth, clustering in cooling granular gas, dynamic heterogeneity in glasses, etc. We also observe that systems do not provide self-averaging proportionate to their sizes [7].

In Ising models, the conserved order-parameter dynamics, where composition of up (A_1 particle) and down (A_2 particle) spins remains fixed during the entire evolution, may be implemented via the standard Kawasaki exchange mechanism [8] where for a Monte Carlo (MC) move interchange of positions between a pair of nearest-neighbor (nn) spins is attempted. A move is accepted or rejected according to the standard Metropolis algorithm [9]. This mimics diffusive transport in solid binary mixture [9]. In our study periodic boundary conditions were applied in both the x and y directions. For $L=16$, 32, and 64, all results were averaged over 1000 independent initial configurations whereas for $L=128$ averaging was done over 40 initial configurations.

In Fig. 1, we present snapshots during the evolution of an Ising system, starting from a 50:50 random mixture of up and down spins, on a square lattice of linear size $L=128$ obtained via MC simulation at temperature $T=0.6T_c$, T_c being the critical temperature. The times at which the shots were taken are mentioned on the figure. While the last snapshot corresponds to a situation when A_1 and A_2 phases are completely separated, the one at $t=4.5\times10^6$ Monte Carlo steps (MCS) represents the situation when finite-size effect began to enter, as will be clear later. Note that all physical

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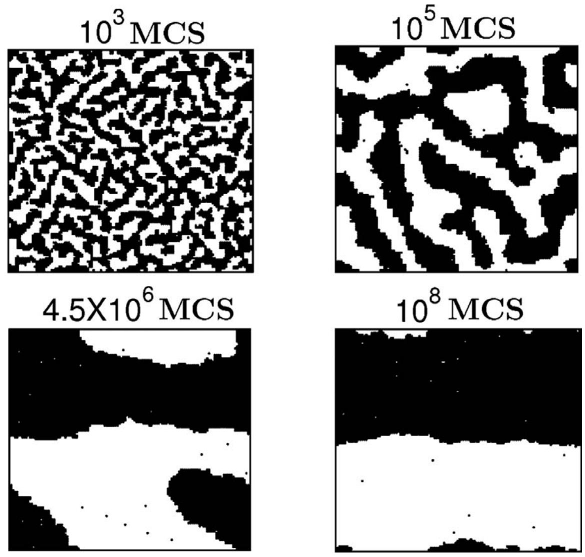

FIG. 1. Evolution snapshots (black$\rightarrow A_1$, white$\rightarrow A_2$) of domain coarsening in a 2D conserved Ising model following a quench from a high-temperature random state to $T=0.6T_c$ for a system of size $L^2=128^2$.

quantities were calculated from the pure domain morphology after eliminating the thermal noise via a majority spin rule where a spin at a lattice site j is replaced by the sign of majority of the spins sitting at j and nn of j.

Figure 2 shows the plot of $\ell(t)$ vs t for $L=32$, 64, and 128, where $\ell(t)$ was calculated from the first moment of the domain-length distribution function [10] $P(\ell_k)$ with the length ℓ_k being the separation between two successive interfaces in the x or y directions. The flat regions of the data sets correspond to the situation when the systems have reached their final equilibrium states so that domains cannot grow further. This limiting value, for the present calculation, comes out to be $\ell_{\max} \simeq L/2$. The last snapshot in Fig. 1 represents such a situation. In the inset of Fig. 2, we demonstrate the scaling behavior of the correlation function, as embodied in Eq. (1), for $L=128$. The data collapse observed upon dividing r by $\ell(t)$ is good starting from as early as $t=10^3$ MCS until $t=4.5\times10^6$ MCS when the finite-size effects begin to appear. Apparently, as is clear from the plot of $\ell(t)$ vs t as well as the scaling behavior of $C(r,t)$ for very extended time and length scale, the size effect is negligible *almost* up to $\ell_{\max}$. However, to make quantitative statements an appropriate scaling analysis is called for.

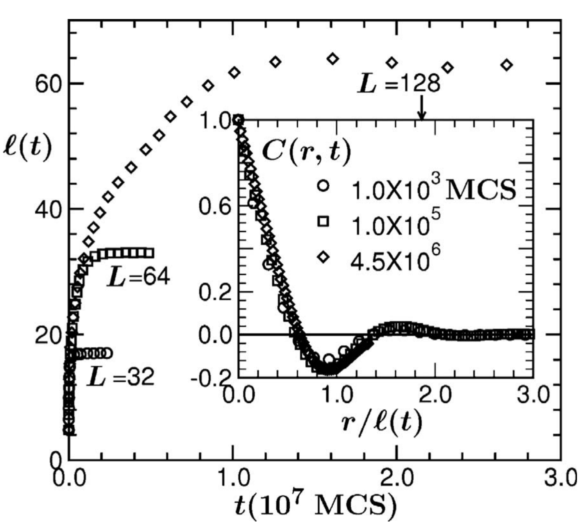

FIG. 2. Plot of average domain size as a function of time for three different system sizes $L=32$, 64, and 128, as indicated. The inset shows a scaling plot of $C(r,t)$ vs $r/\ell(t)$ for $L=128$ for the three different times mentioned.

In analogy with critical phenomena [5], one can construct the finite-size scaling ansatz [11] by identifying $\ell(t)$ with the equilibrium correlation length ξ and $1/t$ with the temperature deviation from the critical point. At this stage we introduce a length $\ell(t_0)$ corresponding to the time t_0 since the quench at which the system becomes unstable. In all subsequent discussions we quantify the growth,

$$\ell(t) = \ell(t_0) + At^{\alpha}, \tag{4}$$

by measuring time t with respect to the reference value t_0. Note that slightly poor data collapse in Fig. 2 is primarily because $C(r,t)$ should have been plotted as a function of $r/[\ell(t)-\ell(t_0)]$ not $r/\ell(t)$. But $C(r,t)$ contains information about $\ell(t)$ and subtracting the influence of $\ell(t_0)$ is a rather challenging task.

Equation (4) is valid in absence of any finite-size effect. However, when $\ell(t)$ is comparable to $\ell_{\max}$, finite-size effects comes in and Eq. (4) needs to be modified by accounting for the size effect via

$$\ell(t) - \ell(t_0) = y(x)t^{\alpha}. \tag{5}$$

Here, $y(x)$ is a scaling function, independent of the system size, which depends upon the scaling variable

$$x = [\ell_{\max} - \ell(t_0)]/t^{\alpha}. \tag{6}$$

Combining Eqs. (4)–(6), one can write down the limiting behavior for $x \rightarrow 0$ ($t \rightarrow \infty$, $\ell_{\max} < \infty$) as

$$y(x) \approx x \tag{7}$$

and for $x \rightarrow \infty$ ($\ell_{\max} \rightarrow \infty$) as

$$y(x) = A. \tag{8}$$

In Fig. 3, we plot $y=[\ell(t)-\ell(t_0)]/t^{\alpha}$ as a function of $x/(x+x_0)$ with $x_0=5$, for which we have varied α and $\ell(t_0)$ to achieve optimum collapse of the data from different system sizes. This is obtained for the choices $\ell(t_0=20) \simeq 3.6$ and $\alpha=0.334$. Note that $\ell(t_0)$ in our analysis is a bare length, independent of time, while the scaling behavior [Eq. (5)] will be obtained when this is chosen appropriately. These numbers, as expected, provide a constant value of $y(x)$ in the region unaffected by finite system size, which should be identified with the growth amplitude A. The arrow in Fig. 3 marks the location where $y(x)$ starts deviating from its constant value, signaling the appearance of finite-size effects at

$$\ell(t) = (0.75 \pm 0.05)\ell_{\max}. \tag{9}$$

This value is substantially larger than previous expectations. Note that the snapshot at 4.5×10^6 MCS in Fig. 1 corresponds to this borderline.

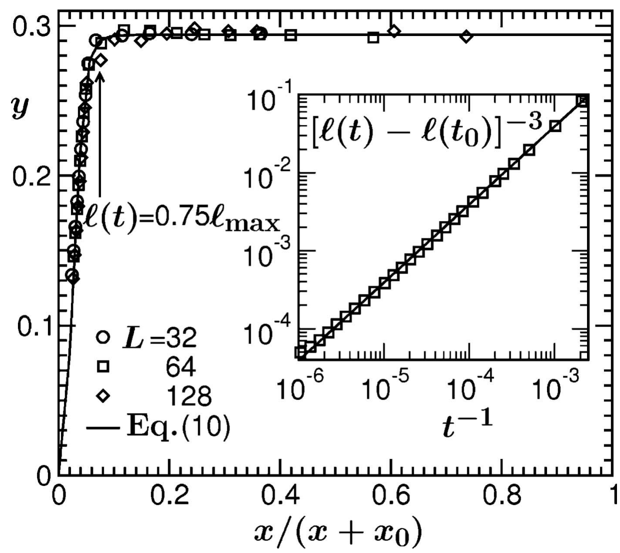

FIG. 3. Finite-size scaling plot of y, with $\ell(t_0=20)\simeq 3.6$ and $\alpha=0.334$, as a function of $x/(x+x_0)$ with $x_0=5$. The continuous curve is a fit to Eq. (10) with the parameters mentioned in the text. The arrow roughly marks the appearance of finite-size effects. Inset: $[\ell(t)-\ell(t_0)]^{-3}$ vs t^{-1} for $L=64$. The straight line has slope 39.

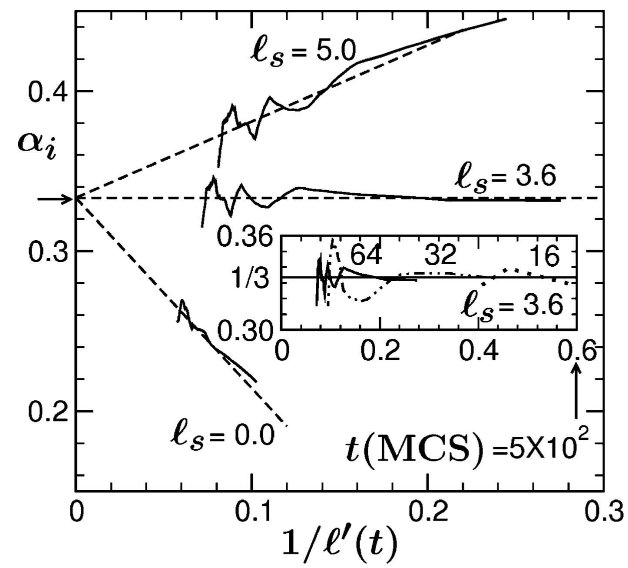

FIG. 4. Plot of the instantaneous exponent α_i as a function of $1/\ell'(t)$ for three different choices of ℓ_s for $L=64$. The dashed straight lines have slopes -1.19, 0, and 0.49, respectively. The arrow on the ordinate marks the value $\alpha=1/3$. Inset: α_i vs $1/\ell'(t)$ for $\ell_s=3.6$ and $L=16$, 32, and 64.

Considering the limiting behavior [Eqs. (7) and (8)], we construct the following functional form, namely,

$$y(x) = Ax/[x + 1/(p + qx^{\beta})]. \quad (10)$$

The continuous line in Fig. 3 is a fit to this form with $A \simeq 0.295$, $p\simeq 3$, $q\simeq 6400$, and $\beta=4$, which has the limiting behavior $(x\to\infty)$ $y(x)\approx A[1-fx^{-5}]$. Of course, an exponential correction term cannot be ruled out. This may be compared with much slower convergence of similar scaling function in dynamic critical phenomena [12]. In the inset of Fig. 3, we plot $[\ell(t)-\ell(t_0)]^{-3}$ vs t^{-1} for $L=64$, on a logarithmic scale to bring visibility to a wide range of data. The continuous line there is a plot of the form ax with $a\simeq 39=1/A^3$. The linear behavior of data starting from very early times justifies the introduction of $\ell(t_0)$.

Next, to further substantiate our claim on negligible correction to scaling as well as recommendations for using small systems, we introduce a length ℓ_s by writing

$$\ell'(t) = \ell(t) - \ell_s = [\ell(t_0) - \ell_s] + At^{\alpha} \quad (11)$$

and define an instantaneous exponent [6] $\alpha_i = d[\ln \ell'(t)]/d[\ln t]$ to find

$$\alpha_i = \alpha\{1 - [\ell(t_0) - \ell_s]/[\ell'(t)]\}. \quad (12)$$

In Eq. (11), the finite-size scaling function $y(x)$ is omitted since, at this point, we are interested in the time regime unaffected by finite system sizes. According to Eq. (12), when α_i is plotted as a function of $1/\ell'(t)$, for $\ell'(t)>0$ one expects linear behavior with a y intercept equal to α. Note that this linear convergence was earlier [6] attributed to strong corrections to scaling. Figure 4 shows such plots for $\ell_s=0$, 3.6, and 5.0, as indicated. The dashed lines have y intercept $\alpha=1/3$ and slopes $m=-[\ell(t_0)-\ell_s]/3$. The consistency of actual data with the dashed lines is remarkable, particularly, the behavior of α_i for $\ell_s=\ell(t_0=20)\simeq 3.6$ again speaks to the choice of $\ell(t_0)$ and strongly indicates that the LS scaling regime is realized very early. Also notice the inset for α_i vs $1/\ell'(t)$ with $\ell_s\simeq 3.6$ for varying system sizes $L=16$, 32, and 64.

This result is in strong disagreement with earlier [6] understanding of domain coarsening in two-dimensional (2D) conserved Ising models that α is strongly time dependent, the LS value being recovered only asymptotically as $\ell(t\to\infty)\to\infty$. The route to this finite-time correction was thought to be an additional term $\propto 1/\ell(t)^3$ in Eq. (3), accounting for an enhanced interface conductivity. Note that a term $\propto 1/\ell(t)^3$ in Eq. (3) could also be motivated by introducing curvature dependence in σ via $\sigma/[1+2\delta/\ell(t)]$, δ being the Tolman length [13]. However, our observation of negligible correction to the exponent, starting from early times, is consistent with the growing evidence that the Tolman length is absent in a symmetrical situation [14]. Thus only corrections of higher orders are expected. Essentially, the misunderstanding about the strong $\ell(t)$ dependence in α was due to the presence of a time-independent length in $\ell(t)$ which our analysis subtracts out in appropriate way.

The appearance of growing oscillations in α around the mean value, as seen in Fig. 4, was also noted by Shinozaki and Oono [15]. In a finite system, as time increases, for an extended period of times two large neighboring domains of the same sign may not merge, thus lowering the value of α_i, after which their meeting brings drastic enhancement of α_i. This character is in fact visible in the direct plot of $\ell(t)$ for $L=128$ in Fig. 2. This oscillation could be a source of error if one obtains α from least-squares fitting.

In conclusion, this Rapid Communication reports a comprehensive finite-size scaling analysis of domain coarsening in a two-dimensional phase separating system. Our accurate and appropriate estimate of the growth exponent, for which we quote 0.334 ± 0.004, is almost coincident with the expected LS value $\alpha = 1/3$, within small error bars. As opposed to the earlier conclusions, the correction appears to be very small, thus LS scaling behavior is obtained very early. Small primary finite-size effects is surprising but welcome message, suggesting a strategy of avoiding large systems and, rather, focusing on accessing long time scales which often is necessary for systems exhibiting multiple scaling regimes. Our observation should be contrasted with an earlier study by Heermann *et al.* [11] that reports very strong finite-size effects. The latter study was based on an extreme off-critical composition and should not be considered to have general validity. Even though size effects may be situation and system dependent, recent study [16] of phase separation in a binary fluid at critical composition provides good agreement with the findings of the present work. Nevertheless, one should be prepared to encounter stronger size effects in more complicated situations, e.g., in systems generating anisotropic patterns [3]. In line of this work many earlier studies on domain coarsening may need to be revisited for proper understanding which was not gained because of lack of reliable methods of analysis. In a later paper we will address similar issue for nonconserved dynamics.

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