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Abstract. We study kinetics of phase segregation in multicomponent mixtures via Monte Carlo simulations of the q-state Potts model, in two spatial dimensions, for $2 \leq q \leq 20$. The associated growth of domains in finite boxes, irrespective of q and temperature, can be described by a single universal finite-size scaling function, with only the introduction of a nonuniversal metric factor in the scaling variable. Our results show that although the scaling function is independent of the type of transition, the q-dependence of the metric factor hints to a crossover at $q = 5$ where the type of transition in the model changes from second to first order.

1. Introduction

The nonequilibrium process of phase separation of a mixture into its components, following a quench inside its demixing region, happens through the growth of clusters or domains of like species, once the system becomes thermodynamically unstable [1, 2]. The characteristic dynamic length scale of the process, i.e., the average domain size ℓ, generally follows a power law with time t, viz., $\ell(t) \sim t^{\alpha}$, α being the growth exponent. Typically, α depends on the intrinsic dynamics of the system, e.g., in solid mixtures, where the dynamics is diffusive, the value of α is $1/3$, referred to as the Lifshitz-Slyozov (LS) growth law [3]. To understand segregation phenomena in two-component solids, the spin-1/2 Ising Hamiltonian has been extensively studied via Monte Carlo (MC) methods [4, 5, 6, 7]. Earlier studies reported estimates for α that are significantly lower compared to the LS value. Later, results obtained via certain extrapolation of the finite-time exponents were explained by arguing that the LS exponent can be realized only when $t \to \infty$ [8]. Naturally, this suggests that there exist corrections to the scaling law at finite time. More recently, however, it has been demonstrated [9, 10, 11], via appropriate finite-size scaling (FSS) analyses, that the LS growth is realized even at finite times, ruling out [6, 9, 10, 11] the presence of the above mentioned strong corrections. This motivated us to apply such FSS analyses to the study of kinetics in mixtures having more than two species, for which the number of studies is limited [12, 13, 14].

Basic physics of a multicomponent mixture can be captured by the q-state Potts model. For nearest-neighbor interaction the Hamiltonian for this model is (σ_i being the state at site i) [15]

$$H = -J \sum_{\langle ij \rangle} \delta_{\sigma_i,\sigma_j}; \;\; \sigma_i = 1, 2, \ldots, q, \tag{1}$$

where $\delta_{m,n}$ is the Kronecker delta function and $J > 0$ is the interaction strength. For $q = 2$, the Hamiltonian in Eq. (1) reduces to the Ising one, apart from a prefactor. This model undergoes a phase transition which is of second order for $q \leq 4$ and beyond that it is of first order [15]. The transition temperature of the model is given by $T_c(q) = J/\left[k_B \ln(1+\sqrt{q})\right]$, with k_B being the Boltzmann constant. In this article, we extend our previous work [16] on the segregation kinetics in multicomponent mixtures to higher values of q via MC simulations of the above model, subsequent analyses of the data being performed via a FSS method.

2. Methods

We perform canonical MC simulations [17] in space dimension $d = 2$, on square lattices, with periodic boundary conditions. Since the number of particles of each type, during phase separation, is constant, the simulation is conducted via the standard Kawasaki dynamics [17]. In this method, a trial move is performed by interchanging positions of two nearest-neighbor particles, chosen at random. The standard Metropolis criterion is used to accept such moves [17]. Our unit of time is one MC step (MCS) that consists of L^2 attempted moves where L is the linear dimension of the square lattice. An initial configuration, mimicking a high-temperature homogeneous mixture, consists of a random arrangement with equal concentration of all spin or particle states. Finally, the simulations are run with $L = 128$, at quench temperatures $T < T_c(q)$. In our simulations the unit of T is J/k_B, and we set both J and k_B to unity. All quantitative results are presented after averaging over 50 independent runs.

3. Results

Evolution of systems, following temperature quenches, are depicted in Fig. 1(a), where we show snapshots from two different times, for a small q (= 3) as well as a large q (= 20). For high q, especially at early times, there exists a large number of point defects which are defined as the meeting point of three or more states. However, at late times, even for q as high as 20, the one-dimensional line defects or domain walls are the majority, and therefore, the growth is not expected to be affected by those point defects.

Structural self-similarity, that is generally associated with coarsening phenomena, is reflected in the superposition properties of a number of morphology related functions such as the two-point equal-time correlation, the structure factor, and the size distribution function of the domains [1]. For each of these functions, data from different times t can be collapsed onto appropriate master curves that are independent of t [1]. For example, the distribution function, $P(\ell_d, t)$, of domain lengths ℓ_d, obeys the scaling $P(\ell_d, t) = \ell(t)^{-1}\tilde{P}[\ell_d/\ell(t)]$, with $\tilde{P}$ being a master function [1, 2]. In this work we rely on this scaling for consistent self-similarity during growth [16] and obtain the average domain size as $\ell(t) = \overline{\ell}_d = \int d\ell_d \; \ell_d P(\ell_d, t)$, where ℓ_d is measured from the distance between a pair of neighboring domain boundaries, along any Cartesian axis. To circumvent the effect of thermal noise in estimating ℓ_d, we apply a majority spin rule that provides pure, zero temperature like, domain structures [10]. The dependence of ℓ on t, for a few values of q, at $T = 0.7T_c(q)$, are shown in Fig. 1(b). The inconsistency [16] of the data with the expected LS growth (shown by the solid line) increases with q. Such discrepancy was previously [8, 14] attributed to the presence of finite-time corrections and it was believed that the LS growth can only be realized for $\ell(t) \to \infty$. In the following, via application of FSS, we show that those corrections are negligible and the LS law can be observed at finite times, even for very large q.

By incorporating an initial domain size ℓ_0, which is the average length at time t_0 (measured from the moment of quench) when the mixture renders unstable to fluctuations, we quantify the growth as [9, 10, 18, 11]

$$\ell(t) = \ell_0 + A\,(t - t_0)^{\alpha}\,. \tag{2}$$

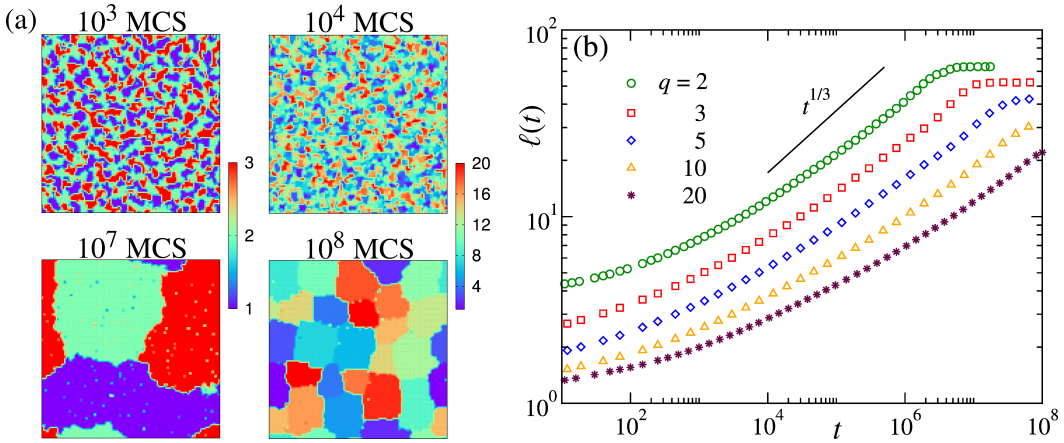

Figure 1. (a) Snapshots showing domain coarsening in the $d = 2$ Potts model with $q = 3$ (left) and $q = 20$ (right) at $T = 0.7T_c(q)$, following quenches from randomly mixed phases at high temperature. Color coding for different states are separately shown for each of the q values. (b) Log-log plots of the characteristic length $\ell(t)$ versus t, for five values of q, at $T = 0.7T_c(q)$. The solid line represents the LS growth.

Recalling FSS in equilibrium critical phenomena [19, 20], one uses the correspondence $\ell(t) - \ell_0 \hat{=} \xi$ and $1/(t - t_0) \hat{=} |T - T_c|$, to write [18]

$$Y(y) \quad = \quad \frac{\ell(t) - \ell_0}{\ell_{\rm max} - \ell_0}, \text{ choosing } y = \frac{(\ell_{\rm max} - \ell_0)^{1/\alpha}}{(t - t_0)}. \tag{3}$$

Note that $\ell_{\rm max}$ ($\sim L$) is the saturation length, i.e., the largest domain size one can access in a finite system of size L [9, 16]. From Eqs. (2) and (3), it transpires that in the growth regime ($y \to \infty$) $Y(y) \sim y^{-\alpha}$, and when one approaches the finite-size limit ($y \to 0$) $Y(y) \to 1$. During the FSS analysis α is tuned, with the objective of superimposing data from different L optimally. For the best collapse, Y should obey the above limiting forms. We obtained values of ℓ_0 (or t_0) from $\alpha_i = \frac{d \ln \ell(t)}{d \ln t}$, the finite-time exponents [8], versus $1/\ell(t)$ data (see Ref. [16] for details), and so, these are not adjustable parameters. For brevity, we do not present any result on FSS for a fixed q, instead move onto capturing the universality in the scaling for different q.

For that purpose we modify the scaling variable y by rewriting it as [16]

$$y_q = f_q \frac{(\ell_{\rm max} - \ell_0)^{1/\alpha}}{(t - t_0)}, \text{ where } f_q = \left[\frac{A(q = 2)}{A(q)}\right]^{1/\alpha}. \tag{4}$$

The metric factor f_q is related to the amplitude A in Eq. (2), which is a function of q. We have $Y = 1$, as $t \to \infty$, for all q. Thus, without f_q, for different values of q, the $Y(y)$ in Eq. (3) would only have horizontal separation from each other. Here, treating $q = 2$ as reference, to obtain an optimum collapse, along with the $Y(y_q) \sim y_q^{-\alpha}$ behavior, we adjust f_q for data from different q. Reasonably good collapse of data, that is obtained by fixing $\alpha = 1/3$ [shown in Fig. 2(a)], confirms not only the LS growth from very early time for all q, but also the fact that the growth dynamics, irrespective of q, is describable by a single universal FSS function. This combined fact further implies that finite-size effects are also the same for all q. This is consistent with the report of very robust universality in finite-size effects in coarsening phenomena, observation made from studies of other systems [11, 18]. Existence of such universal FSS function got reported first in connection with equilibrium critical phenomena [21, 22] and has recently been

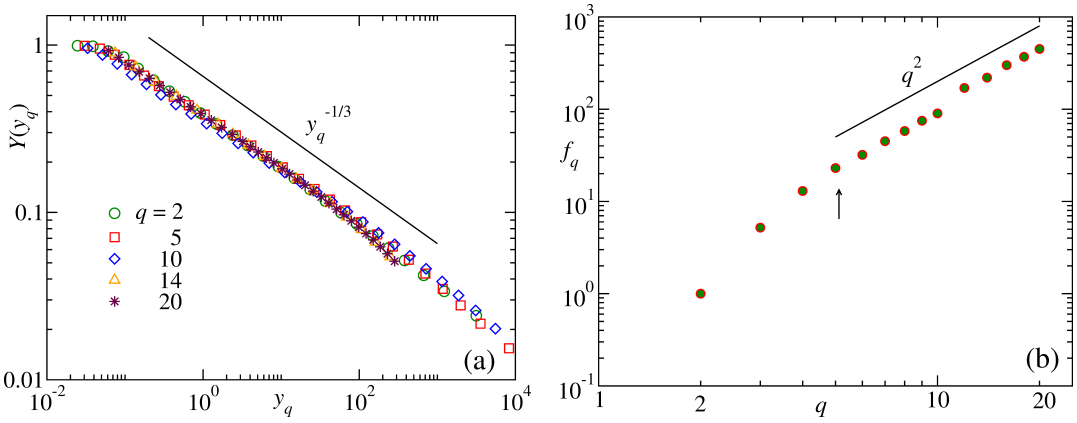

Figure 2. (a) Illustration of the universality of the FSS function, $Y(y_q)$, for the domain growth for different q at $T = 0.7T_c(q)$, extending Fig. 10 of Ref. [16] to larger values of q. Here $Y(y_q)$ is shown versus the scaling variable y_q defined in (4) that contains a nonuniversal metric factor f_q. The solid line corresponds to the expected $Y(y_q) \sim y_q^{-\alpha}$ behavior for $y_q \gg 0$. (b) Log-log plot of f_q as a function of q. The solid line represents q^2 behavior. The arrow points towards $q = 5$.

adapted to understand the kinetics of polymer collapse [23, 24]. As evident, even though the scaling function is universal, f_q is nonuniversal. Its variation as a function of q, plotted on a log-log scale in Fig. 2(b), shows a crossover at $q = 5$, the onset point of first-order transitions in the $d = 2$ Potts model. The post-crossover behavior of f_q is quite consistent with q^2, shown by the solid line. More comprehensive studies are essential to validate this observation [25].

For the temperature dependence of the growth too, one can design a similar scaling apparatus, by replacing y_q with [16]

$$y_T = f_T \frac{(\ell_{\max} - \ell_0)^{1/\alpha}}{(t - t_0)}, \text{ where } f_T = \left[\frac{A(T = 0.7\,T_c)}{A(T)}\right]^{1/\alpha}. \tag{5}$$

Again, one needs to look for the optimum collapse of data, in this case from different T, for a fixed q, along with the corresponding $Y(y_T) \sim y_T^{-\alpha}$ behavior in the early time regime. Here also fixing α to 1/3 yields reasonable quality of collapse of data for $T \in [0.5T_c(q), 0.85T_c(q)]$, confirming the temperature independence of the LS growth. For details of this exercise and corresponding scaling plots see Ref. [16].

Finally, combining Eqs. (4) and (5) one can introduce a "super"-scaling variable [16]

$$y_s = f_q f_T \frac{(\ell_{\max} - \ell_0)^{1/\alpha}}{(t - t_0)}. \tag{6}$$

Using y_s it can be easily shown that the FSS function is not only universal but rather superuniversal. This fact is nicely demonstrated in Fig. 3 where the scaling plots coming from data for different q and T are made to collapse onto a single master curve, along with the realization of $Y(y_s) \sim y_s^{-\alpha}$ behavior.

4. Conclusion

In this paper, we have extended our finding [16] of a universal FSS function for the kinetics of phase separation in the two-dimensional q-state Potts model to higher values of q (up to $q = 20$). Although there exist many more point defects for higher q, the observation of universality of the FSS function, for all q, along with the Lifshitz-Slyozov behavior, suggests that the growth is

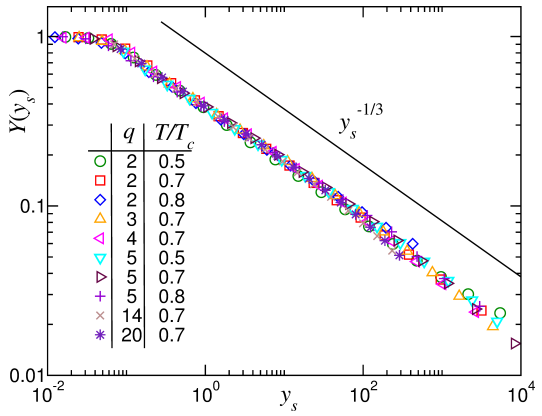

Figure 3. Plot elucidating the fact that domain coarsening in the q-state Potts model is describable by a superuniversal finite-size scaling function $Y(y_s)$, independent of q and the quench temperature T. The solid line has the power-law form $Y(y_s) \sim y_s^{-\alpha}$.

indeed driven by domain wall shrinking. Interestingly, we have observed signature of a crossover in the behavior of the metric factor f_q at $q = 5$ that coincides with the onset point for first-order transitions in the Potts model. A thorough investigation of this connection is needed. It remains to be seen if an analogous study with nonconserved dynamics provides similar information [25].

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