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Coarsening in the Potts model: out-of-equilibrium geometric properties

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Abstract. Geometric properties of polymixtures after a sudden quench in temperature are studied through the q-states Potts model on a square lattice, and their evolution with Monte Carlo simulations with non-conserved order parameter. We analyse the distribution of hull enclosed areas for different initial conditions and compare with exact and numerical findings for the $q = 2$ (Ising) case.

1. Introduction

Curvature-driven ordering processes, in non conserved scalar order parameter systems, underlie many interesting cellular growth processes and are of both theoretical and technological importance, applications including foams [1], cellular tissues [2], superconductors [3], magnetic domains [4, 5], liquid crystals [6], adsorbed atoms on surfaces, *etc.* These systems are spatially divided in many coexisting domains, in which one of the q possible spin orientations dominates, separated by interfaces whose local velocity is ruled by the Allen-Cahn equation, thus being proportional to the local curvature, $v = -(\lambda/2\pi)\kappa$, where λ is a temperature and q-dependent dimensional constant related with the surface tension and mobility of a domain wall and κ is the local curvature. The sign is such that the domain wall curvature is diminished along the evolution. In $d = 2$ the time dependence of the area contained within any finite domain interface (the hull) on a flat surface is obtained by integrating the velocity around the hull and using the Gauss-Bonnet theorem:

$$\frac{dA_n}{dt} = \begin{cases} -\lambda, & q = 2 \\ \dfrac{\lambda}{6}(n-6), & q > 2 \end{cases} \tag{1}$$

where n is the number of sides (or, equivalently, vertices). At each one of these vertices the tangent vector to the surface has a turning angle, that are absent for $q = 2$ (since in this case each domain is surrounded by a single neighbour). Notice that in both cases, the rate is size independent [7, 8], while for $q = 2$ it does not depend on the number of sides.

For $q = 2$, the growth law is homogeneous and all hull enclosed areas decrease with the same rate, what has led us to exactly obtain [8] the number of hull-enclosed areas per unit system

area, in the interval $(A, A + dA)$. For example, if one takes as initial states ($t = 0$), equilibrium configurations at T_c, whose distribution is exactly known for $q = 2$ [9], $n_h(A, 0) = c_h^{(2)}/A^2$ with $c_h^{(2)} = 8\pi\sqrt{3}$, the distribution at any $t > 0$ is

$$n_h(A, t) = \frac{c_h^{(2)}}{(A + \lambda_h t)^2}, \tag{2}$$

that compares extremely well with simulation data for the Ising model on a square lattice [8, 10, 11]. Moreover, the above equation scales as $n(A, t) = t^{-2} f(A/t)$, in accordance with the scaling hypothesis. Although this is usually only a hypothesized, but well-established feature, for the $q = 2$ model it can be obtained from first principles [8]. For a quench from infinite temperature, on the other hand, the initial distribution corresponds to the one of the critical random continuous percolation [8, 10]. This observation is an essential ingredient to understand the fact that, and obtain the probability with which, the system attains a striped frozen state at zero temperature (see [12] and references therein). Interestingly, on a square lattice, the initial state does not correspond to the random percolation critical point but the coarsening evolution gets very close to it after one or two Monte Carlo steps. Therefore, although the analytical results of Ref. [8] were obtained with a continuous description, a priori not guaranteed to apply on a lattice, they do describe the coarsening dynamics of the discrete Ising model with remarkable accuracy.

For $q > 2$, whether a cell grows, shrinks or remains with constant area depends on its number of sides being, respectively, larger than, smaller than or equal to 6, what is known as the von Neumann's law. Therefore, one cannot write a simple relation to link the area distribution at time t to the one at the initial time $t = 0$ and the distribution might get scrambled in a non-trivial way during the coarsening process (for example, when a domain disappears, the number of sides of the neighboring domains changes, along with their growth rate) [13]. Nonetheless, the system again evolves to a scaling state in which the domain morphology is statistically the same at all times when lengths are measured in units of $R(t)$, a single characteristic growing length scale, in accordance with the scaling hypothesis.

In this paper we briefly compare the cases $q = 2$ and $q > 2$, in particular when the initial state was equilibrated at $T = T_c$. We first present the $d = 1$ case and then the much richer two dimensional one, reviewing some of the results already published in Refs. [8, 13]. Besides completeness, it is interesting to compare the uni and two dimensional cases as they strongly differ.

2. Coarsening in $d = 1$

The Hamiltonian in this case is

$$\mathcal{H} = -J \sum_i \delta_{s_i, s_{i+1}}, \tag{3}$$

where $s_i = 0, ..., q - 1$ and $J > 0$. We measure the domain length distribution at time t, $n(\ell, t)$ ($1 \leq \ell \leq L$) after quenching the system from $T_0 \to \infty$ to the final, working temperature, $T = 0$. There is no finite static critical temperature and the system orders ferromagnetically only at $T = 0$. The completely disordered initial condition starts evolving in a coarsening regime in which regions of finite length order. Differently from the higher dimensional case where domain growth is driven by interfacial tension, in $d = 1$ coarsening is driven by the diffusion of domain walls and annihilation when they meet. At this point when a domain disappears, the two neighboring domains always coalesce if $q = 2$. This may not be the case for $q > 2$ and becomes less probable as q increases. Thus, the average length size of the domains, $\langle \ell \rangle$, grows faster the smaller the value of q. Indeed, the growth law is $\langle \ell \rangle = q\sqrt{\pi t}/(q - 1)$ [14, 15], where the $t^{1/2}$ behaviour is expected from the diffusive interface motion.

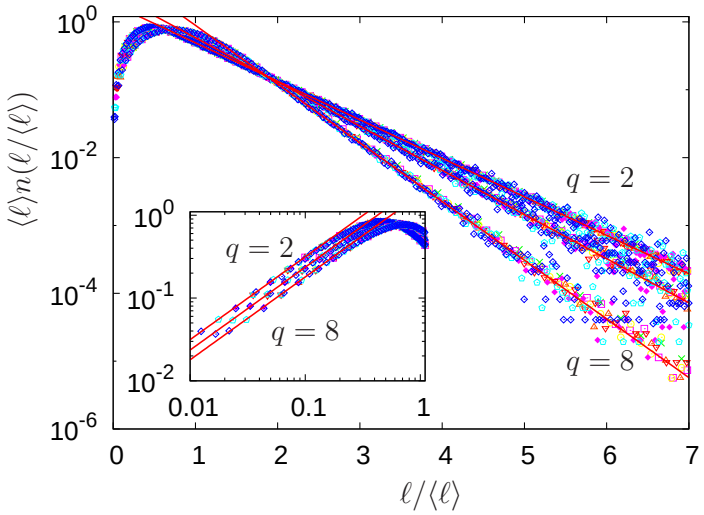

Figure 1. Cluster length distribution for the unidimensional Potts model with $q = 2$, 3 and 8 versus the rescaled length, $\ell/\langle\ell\rangle$. The qualitative behaviour is the same, linear for small lengths and exponential at large ones. The (red) lines are analytical predictions of Derrida and Zeitak [15], eq. (5) with (A_q, B_q) equal to $(1.306, 0.597)$, $(1.500, 0.963)$ and $(1.993, 1.876)$ for $q = 2$, 3 and 8, respectively. The system is 10^5 large and averages were taken over 1000 samples. Data corresponds to times from $t = 2^2$ to 2^9.

During the coarsening regime, the distribution of domain sizes obeys the scaling behaviour

$$n(\ell, t) = \langle\ell(t)\rangle^{-1} f\left(\frac{\ell}{\langle\ell(t)\rangle}\right). \tag{4}$$

At zero working temperature the universal function $f(x)$ is given by [14–17]

$$f(x) = \begin{cases} \dfrac{\pi q x}{2(q-1)} & x \ll 1\,, \\ \exp(-A_q x + B_q) & x \gg 1\,, \end{cases} \tag{5}$$

where the constants are known exactly [15]. In Fig. 1 we show, for $q = 2$, 3 and 8, that the above equations fully agree with numerical simulations (the $q = 2$ case was previously presented in Ref. [10]). In all cases the initial state has null correlations, all spins being fully uncorrelated, what seems to be the key ingredient for the exponential tail in the distribution. As we will see in the next section, the $q = 2$ case, starting from infinite temperature, is an exception to such behaviour.

3. Coarsening in $d = 2$

The detailed evolution of the system during the coarsening dynamics depends on the correlations already present in the initial state. Below we show the behaviour when such correlations are either absent ($T_0 \to \infty$) or long-ranged ($T_0 = T_c$ for $q \leq 4$). In the latter case, since the thermodynamic transition also corresponds to a percolation transition in $2d$, the initial state already presents one spanning cluster at $t = 0$. On the other hand, for short-range initial correlations, such spanning domains are either formed very fast (e.g. in the case $q = 2$ with $T_0 \to \infty$), or not formed at all. We should emphasize the exceptionality of the $q = 2$ case: having the highest concentration of a single species at $T_0 \to \infty$, the proximity with the

percolation critical point strongly affects the system's evolution [8]. Indeed, the hull-enclosed area distribution (geometric domains present an analogous behaviour [10]) becomes power-law in a couple of steps, and the effective initial condition is given by $n_h(A,0) = 2c_h^{(2)}/A^2$ [9]. Power-laws are also the initial distributions for $T_0 = T_c$ for $q \leq 4$ and generally given by (the prefactor is different from the previous case)

$$n_h(A,0) = \frac{(q-1)c_h^{(q)}}{A^2}. \tag{6}$$

Notice that, unless for $q = 2$, the value of $c_h^{(q)}$ is not known exactly, although they are all close to each other.

For $2 \leq q \leq 4$, the Potts model presents a continuous transition, and one could imagine that their non equilibrium coarsening phenomenology would be similar as well. Indeed, the equal time correlation function seems to share the same universal scaling function and the related correlation length grows with the same power of time, $t^{1/2}$. There are, however, fundamental differences. Differently from the $q = 2$ case, that presents a percolating domain with probability almost one as early as $t = 2$ after the quench [8, 10], the $q > 2$, $T_0 \to \infty$ initial condition is sufficiently far from critical percolation that the system remains, at least in the time window of our simulations, distant from the percolation threshold (in spite of the largest domain steadily, but slowly, increasing with time). In this regard, the $q = 2$ case is the exception, while the $q = 3$ and 4 are similar. As the system evolves after the quench, the distribution keeps memory of the initial state, that corresponds to random percolation with occupation probability $p = 1/q$. And, by not getting close to a critical point, the distributions do not become critical and, as a consequence, do not develop a power law tail, as illustrated in Fig. 2 for $q = 3$ and $T_0 \to \infty$. There is, however, an A^{-2} envelope that is a direct consequence of dynamical scaling, present also for other values of q [13].

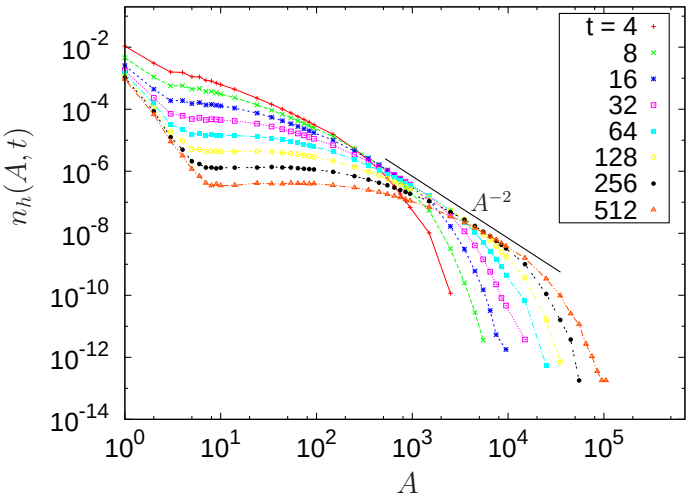

Figure 2. Hull-enclosed area distribution at several times (given in the key) after a quench from equilibrium at $T_0 \to \infty$ to $T_f = T_c/2$ in the $q = 3$ case. Analogous distributions are obtained for $q > 4$ and $T_0 \to \infty$ (not shown). The declivity of the envelope is -2 as a consequence of the scaling obeyed by the distribution. Figure from Ref. [13].

The collapsed distribution of hull-enclosed areas after a quench from $T_0 = T_c$ to $T_f = T_c/2$ for $q = 3$ is shown in Fig. 3. Although for $q = 2$ this distribution conserves its form during

the coarsening regime due to an overall advection to the right as domains increase in size, for $q > 2$ there is a dependence on the number of sides in von Neumann's equation, some domains increase while other decrease in size, and thus there is no obvious reason for the distribution at $t > 0$ to keep its initial power-law form, eq. 6. Remarkably, the general behavior is similar to the $q = 2$ case, in which the collapse of curves for different times onto a single universal function demonstrates the existence of a single length scale that, moreover, follows the Allen-Cahn growth law, $R(t) \sim t^{1/2}$. We can make a mean-field-like approximation and replace the number of sides in the von Neumann equation (1) by a constant mean, $n \to \langle n \rangle$. Using Eq. (6) and the results in Refs. [8, 10], the hull-enclosed area distribution for $q \leq 4$ becomes

$$n_h(A,t) = \frac{(q-1)c_h^{(q)}}{\left(A + \lambda_h^{(q)} t\right)^2}, \tag{7}$$

that fits very accurately the data using $\lambda_h^{(3)} \simeq 1.4$. The deviations present at small values of A/t are due to thermal fluctuations that are visible in the inset (see [10] for details). In order to test the above approximation, we measured the average change in area, dA/dt, that is, the number of spins included or excluded in those domains that survived during a given time interval. The above rate, from von Neumann's equation, depends on $n - 6$ (both in absolute value and sign), and is different for domains with different numbers of neighbours (except for $q = 2$ where it is constant). However, upon average, there is an effective, constant λ_{eff}. Similarly, only those that have $\lambda_{\text{eff}} \leq 0$ present a power law distribution. Thus, there seems to be a net difference between cases that give a power law distribution function from the ones that do not.

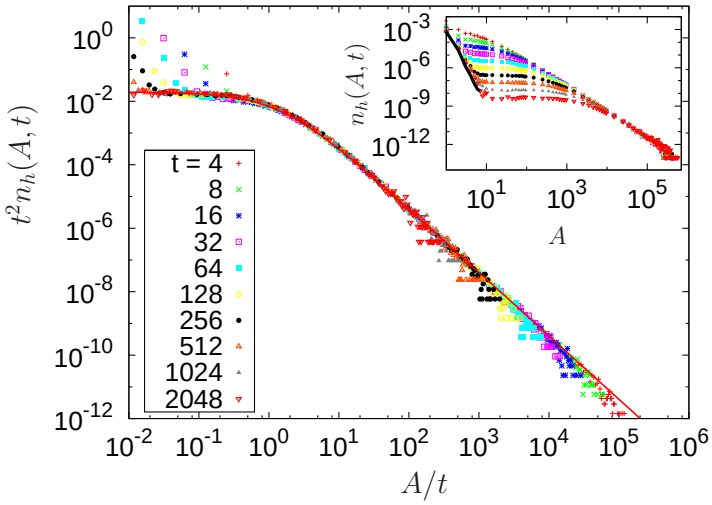

Figure 3. Collapsed hull-enclosed area distributions at several times after a quench from equilibrium at $T_0 = T_c$ to $T_f = T_c/2$, for $q = 3$. The line is Eq. (7) with $\lambda_h^{(3)} \simeq 1.4$. The points at $A/t \ll 1$ that deviate from the scaling function are due to thermal fluctuations. These fluctuations have been independently measured and are depicted as a continuous black line in the inset (notice that their distribution is time independent). Figure from Ref. [13].

4. Conclusions

We studied the Potts model during the coarsening dynamics after a sudden quench in temperature, emphasizing the cases $q = 2$ and 3 that present a continuous transition. Although

the theory developed in Refs. [8, 10] for the Ising model ($q = 2$) cannot be easily extended to $q > 2$, our numerical results show the existence of similarities between both cases. Besides the equilibrium continuous transition, there is a dynamical length scale that grows with $t^{1/2}$ after a sudden quench in temperature and the same universal scaling function for the rescaled correlation function in both cases. Nonetheless, very different are the distributions of dynamic hull-enclosed areas (and geometric domains) evolved from initial states with zero correlation lengths, as those obtained in equilibrium at $T_0 \to \infty$. One expects that the scaling functions of the dynamic distributions will be reminiscent of the disordered state at the initial temperature, with an exponential tail. This is indeed what happens in $d = 1$ and, in $d = 2$, for $q > 2$. The remarkable exception is $q = 2$ (in $d = 2$): the proximity from the percolation critical point, and the subsequent flow to it after the temperature quench, develops a power-law tail in the distribution. For $q = 3$ the initial state is no longer close to any critical point and this does not occur. A further surprise occurs for the distributions after a quench from $T_0 = T_c$. Despite von Neumann's law showing that differently sided domains could either grow or shrink, scrambling the distribution, it still shows a power law, in analogy with the Ising case but without a complete explanation up to now besides a simple mean-field-like argument. Alongside, many questions are still unanswered for this long studied, classic problem and surely many surprises are still awaiting.

Acknowledgments

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