# Correlations and Coarsening in the $q$-State Potts Model

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We study the nonequilibrium dynamics of the $q$-state Potts model following a quench from the high-temperature disordered phase to zero temperature. We calculate, within a Gaussian closure approximation, the time-dependent two-point correlation functions for general $q$. These correlation functions obey dynamic scaling with a length scale $L(t) \sim t^{1/2}$, while the autocorrelation function decays as $L(t)^{-\lambda(q)}$. We also establish a correspondence of this model to the Ising model evolving with a fixed magnetization $(2/q - 1)$. Extensive numerical simulations of the Potts model in two dimensions show good agreement with our theory.

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Coarsening of domains of equilibrium ordered phases, following a quench from the disordered homogeneous phase to a regime where the system develops long-range order, is widely observed in many physical systems such as binary alloys, liquid crystals, magnetic bubbles, Langmuir films, and soap bubbles [1,2]. After the quench, domains of different ordered phases form and grow with time as the system attains local equilibrium on larger and larger length scales. A dynamic scaling hypothesis suggests that at late times the system is left with a single length scale (the linear size of a typical domain) which grows with time as $L(t) \sim t^n$, where $n$ depends on the conservation laws satisfied by the dynamics [1,2]. For systems with only two types of ordered phases (such as a binary alloy or the Ising model), the nonequilibrium coarsening dynamics have been extensively studied experimentally, numerically, and by approximate analytical methods. Comparatively, much less is known when there are more than two ordered phases.

A particular example of the latter class of models is the $q$-state Potts model [3]. For $q = 2$, this corresponds to the Ising model, and there are experimental realizations also for $q = 3, 4, \infty$ [3]. As $q$ increases, the morphology of the coarsening patterns changes from one of large, connected, interpenetrating domains to one of more and more isotropic droplets. The limit $q \to \infty$ is known to correctly describe the evolution of a dry soap froth, or the growth of metallic grains [4]. Most studies of soap bubbles have so far focused on geometrical properties of the froth. For instance, mean-field treatments [5,6] and numerical simulations [4], as well as experiments [7], have addressed issues such as the joint distribution of bubble areas and coordination number. For the Potts model with finite $q$, there have been only numerical studies of the growth law of domains, substantiating the form of the growth law, $L(t) \sim t^{1/2}$ [4,8], and the scaling of the equal-time correlation function [8].

In this Letter, we go beyond mean-field theory and present an approximate analytical way to compute both the equal-time and two-time correlation functions. We establish scaling and calculate the scaling functions as well as the exponent $\lambda(q)$ which describes the temporal decay of autocorrelations [9].

For the Ising model, a continuum description can be based on a coarse-grained order parameter field $\phi(\mathbf{r}, t)$. For later convenience, we choose it to be the "occupation density" which takes values 1 in the bulk of one phase and 0 in the other ones. A suitable Landau free energy describing the ordered phase is $F[\phi] = \int d^d\mathbf{r}[\frac{1}{2}(\nabla\phi)^2 + V(\phi)]$, where the potential $V(\phi)$ has a double-well structure, e.g., $V(\phi) = \phi^2(1-\phi)^2$ with degenerate minima at $\phi = 0, 1$ representing the two ordered phases. The evolution of $\phi(\mathbf{r}, t)$ at zero temperature is described in terms of the model-$A$ Langevin equation [10]

$$\frac{\partial \phi}{\partial t} = -\frac{\delta F}{\delta \phi} = \nabla^2\phi - V'(\phi). \tag{1}$$

Dynamic scaling suggests that, at late times, the equal-time correlation function $\langle \phi(0,t)\, \phi(\mathbf{r},t)\rangle$ scales as $g(r/L(t))$ while the autocorrelation with the initial state $A(t) = \langle \phi(\mathbf{r},0)\, \phi(\mathbf{r},t)\rangle$ decays as $A(t) \sim [L(t)]^{-\lambda}$ [9]. The scaling function $g(x)$ and the exponent $\lambda$ have been estimated both numerically and by approximate analytical methods by several authors [1,2]. Of these approximate methods, a reasonably successful one (at least for model-$A$ dynamics) is due to Mazenko [11]. In what follows, we extend some of these ideas developed for two-phase systems to treat the coarsening of $q$-phase systems.

A suitable description of the $q$-state Potts model may be based on $q$ coarse-grained occupation density fields $\{\phi_l(\mathbf{r}, t);\ l = 1, 2, \ldots, q\}$ such that $\phi_l$ assumes the value 1 in the interior of the $l$th ordered phase and decays continuously to 0 outside. Consequently, inside any "bubble" of one phase, only one of the $\phi_l$'s is close to 1 and the others are all close to 0. We thus require a potential with $q$ degenerate minima at $[1, 0, 0, \ldots, 0]$, $[0, 1, 0, \ldots, 0]$, $\ldots$, $[0, 0, 0, \ldots, 1]$, which prevents two different bubbles from sharing the same position in space. A suitable free-energy functional is [12]

$$F[\{\phi_l\}] = \int d^d\mathbf{r}\left\{\sum_{l=1}^{q}[\tfrac{1}{2}(\nabla\phi_l)^2 + V(\phi_l)] - \lambda_1\left(\sum_{l=1}^{q}\phi_l - 1\right) + \lambda_2\left[\sum_{l=1}^{q}(\phi_l - \tfrac{1}{q})^2 - \frac{q-1}{q}\right]^2\right\}, \quad (2)$$

where $\lambda_1(\mathbf{r},t)$ is a Lagrange multiplier enforcing the constraint $\sum_l \phi_l = 1$, and $\lambda_2$ is a constant of $O(1)$ such that the state $[1/q,\dots,1/q]$ is unstable. Then the equation of motion is

$$\frac{\partial\phi_l}{\partial t} = \nabla^2\phi_l - V'(\phi_l) + \lambda_1 - 4\lambda_2(\phi_l - \tfrac{1}{q}) \times\left[\sum_{l'=1}^{q}(\phi_{l'} - \tfrac{1}{q})^2 - \frac{q-1}{q}\right] \quad (3)$$

and $\lambda_1 = \frac{1}{q}\sum_l V'(\phi_l)$, by requiring $\sum_l \phi_l = 1$ in Eq. (3). We note that this evolution equation has a form similar to that of Eq. (2.10) of Ref. [8].

The two-point correlation function for the $q$-state Potts model is defined as $G(12) = \sum_{l=1}^{q}\langle\phi_l(\mathbf{r}_1,t_1)\,\phi_l(\mathbf{r}_2,t_2)\rangle$, and therefore equals $q\langle\phi_l(\mathbf{r}_1,t_1)\,\phi_l(\mathbf{r}_2,t_2)\rangle$, due to the symmetry between the $q$ phases. Here, "12" is a shorthand notation for the pair of space-time points $(\mathbf{r}_1,t_1)$ and $(\mathbf{r}_2,t_2)$. Due to the isotropy and translational invariance in space, the only spatial dependence of these correlation functions is through $r = |\mathbf{r}_1 - \mathbf{r}_2|$. Denoting the equal-time correlation function ($t_1 = t_2 = t$) by $G(r,t)$, we get from Eq. (3),

$$\frac{1}{2}\frac{\partial G}{\partial t} = \nabla^2 G - q\langle\phi_l(0,t)\{V'(\phi_l(\mathbf{r},t)) - \lambda_1\}\rangle - 4\lambda_2 q\left\langle\phi_l(0,t)[\phi_l(\mathbf{r},t) - 1/q]\times\left[\sum_{l'=1}^{q}\phi_{l'}^2(\mathbf{r},t) - 1\right]\right\rangle. \quad (4)$$

Note that the two-time correlation function satisfies a similar equation.

Our first approximation is to replace $\sum_{l'}\phi_{l'}^2$ by its average $q\langle\phi_l^2\rangle = G(0,t)$ in the third term on the right-hand side of Eq. (4), which becomes exact in the $q\to\infty$ limit. Furthermore, the scaling solution $G(r,t) = g(r/L(t))$ must satisfy $g(0) = 1$, so that we can drop the term $4\lambda_2[G(r,t) - 1/q][G(0,t) - 1]$ so produced. Thus the third term, although important in the evolution of $\phi_l$ since it provides stability to the bubbles, is not crucial in the evolution of the correlation functions, at least in the scaling limit of the large-$q$ model, and also for $q = 2$. Next, using $\sum\phi_l = 1$, we get $\langle\lambda_1\sum\phi_l\rangle = \langle\lambda_1\rangle$ and then, given the symmetry between the $q$ phases, $\langle\phi_l\lambda_1\rangle = (1/q)\langle\lambda_1\rangle = \langle\phi_l\rangle\langle\lambda_1\rangle$. Thus, without approximation, we replace $\lambda_1$ by its average $\langle\lambda_1\rangle$, which is simply a function of time. As a result, Eq. (4) reduces to an equation involving only a single field $\phi_l(\mathbf{r},t)$:

$$\frac{1}{2}\frac{\partial G}{\partial t} = \nabla^2 G - q\langle\phi_l(0,t)\{V'(\phi_l(\mathbf{r},t)) - \langle\lambda_1\rangle\}\rangle. \quad (5)$$

Interestingly, Eq. (5) is also the evolution equation for the two-point correlation in an Ising model evolving with fixed average magnetization $\langle m_0\rangle = 2/q - 1$ (equivalently, with a density of minority "up" spins fixed at $1/q$). The droplet domains of the minority phase in this Ising model would correspond to the bubbles of a particular phase in the Potts model, with the majority phase corresponding to the remaining $(q-1)$ phases. $\langle\lambda_1\rangle$ acts as a time-dependent magnetic field which prevents the minority phase from disappearing at $T = 0$, and keeps the magnetization constant.

Let us first discuss briefly the Mazenko approximation for the Ising model [11]. The order parameter field $\phi(\mathbf{r},t)$ changes quite sharply at the domain walls and the probability distribution of $\phi(\mathbf{r},t)$ is certainly far from Gaussian. However, for nonconserved dynamics, where interfaces move locally while equilibrium is maintained in the bulk, one can consider an auxiliary field $m(\mathbf{r},t)$ which is related to $\phi(\mathbf{r},t)$ via a nonlinear transformation $\phi(\mathbf{r},t) = \sigma[m(\mathbf{r},t)]$. The mapping function $\sigma$ is chosen to be the equilibrium profile of the order parameter field and is determined from $d^2\sigma/dm^2 = V'(\sigma)$, with the boundary conditions $\sigma(m)\to 1$ as $m\to\infty$ and $\sigma(m)\to 0$ as $m\to -\infty$. The auxiliary field $m(\mathbf{r},t)$ can then be interpreted as the distance from the nearest interface and, in contrast to $\phi(\mathbf{r},t)$, varies smoothly across the walls. It may then be reasonable to assume that $m(\mathbf{r},t)$ has a Gaussian distribution.

Since the equation of evolution of the correlation function Eq. (5) involves only a single field $\phi_l$, hereafter simply denoted by $\phi$, it is possible to extend the Mazenko approximation for the usual Ising model to our problem. However, several important differences from the simple Ising case must be noted. First, $\langle\phi\rangle$ is strictly fixed at $1/q$ at all times as opposed to the Ising case where, for a critical quench, $\langle\phi\rangle = \frac{1}{2}$ automatically. This also necessarily implies that the mean of the distribution of $m$ is nonzero. The first and second moments of the Gaussian distribution, $\langle m(t)\rangle = \overline{m}(t)$, $\langle\{m(t) - \overline{m}(t)\}^2\rangle = C_0(t)$ and $\langle\{m(t_1) - \overline{m}(t_1)\}\{m(t_2) - \overline{m}(t_2)\}\rangle = C(12)$, must be determined self-consistently. For example, from the condition $\langle\phi(\mathbf{r},t)\rangle = 1/q$, we get

$$\frac{1}{\sqrt{2\pi C_0}}\int_{-\infty}^{\infty}\sigma(m)\exp[-(m-\overline{m})^2/2C_0]\,dm = 1/q\,.$$

Replacing $\sigma[m,t]$ at late times by the step function $\theta(m)$ (which is 1 for $m > 0$ and 0 for $m < 0$) and thereby neglecting terms that are of lower order in $t$, we get $\overline{m}(t) = -\sqrt{2C_0(t)}\,\mathrm{erfc}^{-1}(2/q)$, where $\mathrm{erfc}(x) = (2/\sqrt{\pi})\int_x^\infty \exp(-u^2)\,du$. Note that for $q = 2$, $\overline{m} = 0$ as expected. For later convenience, let us also define the correlation function $f(12) = C(12)/\sqrt{C_0(1)\,C_0(2)}$ and denote it by $f(\mathbf{r},t)$ when $t_1 = t_2 = t$. Note that $f(0,t) = 1$ and $f\to 0$ as $r\to\infty$.

The second important difference from the simple Ising case is the choice of the mapping function $\sigma[m(\mathbf{r},t),t]$.

The explicit time dependence introduced via $\langle\lambda_1\rangle$ modifies the local equilibrium profile. In fact, since the mean of the field $m(\mathbf{r},t)$ is time dependent, one can expect to get a "sigmoid" shaped solution only in a moving frame, with a velocity suitably determined to neutralize the time dependence introduced via $\langle\lambda_1\rangle$. In fact, this moving frame follows the motion of the local interface. Thus, making the transformation $\mathbf{r}' = \mathbf{r} + a(t)\hat{\mathbf{n}}$ where $\hat{\mathbf{n}}$ is an arbitrary unit vector and $a(t)$ is to be determined, and demanding an equilibrium solution, i.e., $\partial\phi/\partial t = 0$ to leading order in time, we find the appropriate equation for $\sigma[m.t]$:

$$\frac{d^2\sigma}{dm^2} + \frac{da}{dt}\frac{d\sigma}{dm} = V'(\sigma) - \langle\lambda_1\rangle. \tag{6}$$

We now fix $a(t)$ from the condition that the average value on both sides of Eq. (6) should be identical. The average on the right-hand side is zero by definition of $\langle\lambda_1\rangle$. The quantities $\langle d^2\sigma/dm^2\rangle$ and $\langle d\sigma/dm\rangle$ are calculated using the Gaussian property of $m$ and replacing $\sigma(m,t)$ by $\theta(m)$ at late times. This yields $da/dt \approx \overline{m}/C_0$, implying $a(t) \sim \sqrt{C_0(t)} \sim L(t)$, which is expected, since, physically, $L(t)$ is the only length scale remaining at late times. From Eq. (6), $\langle\lambda_1\rangle \sim 1/L(t)$, which can be understood on physical grounds: Local equilibrium of a bubble and its interface requires that the surface tension energy $E_S \sim L(t)^{d-1}$ should balance the magnetic energy $E_M \sim \langle\lambda_1\rangle L(t)^d$. Using Eq. (6) in Eq. (5), the expressions for $\overline{m}$ and $da/dt$, and expressing the derivatives of $\sigma$ with respect to $m$ as derivatives with respect to $f$, we obtain [12]

$$\frac{1}{2}\frac{\partial G}{\partial t} = \nabla^2 G + \frac{1}{C_0(r,t)}Q(f), \tag{7}$$

where $Q(f) = f\partial G/\partial f$ with $G(f)$ given by

$$G(f) = \frac{q}{\sqrt{\pi}}\int_0^\infty dy\, \exp\left[-\left(y + p\sqrt{\frac{2}{1+f}}\right)^2\right] \times \operatorname{erf}\left[\sqrt{\frac{1+f}{1-f}}\,y\right], \tag{8}$$

where $p = \operatorname{erfc}^{-1}(2/q)$. $Q$ is then implicitly a function of $G$. Interestingly, we notice that the form $Q(f) = f\partial G/\partial f$ is identical to that of the Mazenko equation [11] for the critical Ising case, with the exception that $G(f)$ has different expressions in the two cases. However, this seems accidental because in our problem we need to invoke a moving frame and therefore a different profile function satisfying Eq. (6). For $q = 2$ ($c = \frac{1}{2}$, Ising critical), the velocity of the moving frame $da/dt \approx \overline{m}/C_0$ is zero identically, and our expression then reduces to the Mazenko results. The scaling form $G(r,t) = g(r/L(t))$ is a solution of Eq. (7) provided that $C_0(t) \sim L(t)^2$ scales linearly with $t$, giving the expected growth law $L(t) \sim t^{1/2}$. Setting $C_0 \approx 4t/\mu$ for large time, and $x = r/L(t)$, we get

$$\frac{d^2 g}{dx^2} + \left(\frac{d-1}{x} + x\right)\frac{dg}{dx} + \mu Q(g) = 0, \tag{9}$$

which defines a closed eigenvalue equation for $g$. $\mu$ has to be determined by matching the short- and long-distance behaviors of $g(x)$. $\lambda$ is then related to $\mu$ via the relation $\lambda = d - \mu/2$ [11,12].

In the $q \to \infty$ limit, it is possible to solve Eq. (9) analytically. Neglecting terms of $O(1/p^4)$ and using $\operatorname{erfc}(p) \sim \exp(-p^2)/p\sqrt{\pi}$ for large $p$, we find

$$g(f) \approx \frac{1+f}{2}\operatorname{erfc}\left[p\sqrt{\frac{1-f}{1+f}}\right]. \tag{10}$$

Then, expressing the function $Q$ in terms of $g$ itself, we find essentially three regimes. As $g \to 1/q$ (large distance), $Q(g) \approx g - 1/q$, and as $g \to 1$ (short distance), $Q(g) \approx p^2/\pi(1-g)$. In the intermediate regime, $g^* \ll g \ll 1$ where $g^* \sim \ln(q)/q$, $Q(g) \approx p^2 g/2$. First consider the small $x$ behavior of Eq. (9). Using $Q(g) \sim p^2/\pi(1-g)$, we find that $g(x) \to 1 - p\sqrt{\mu/\pi(d-1)}\,x$, the cusp reflecting the presence of sharp interfaces. This reproduces Porod's law [13], namely, that the structure factor scaling function $F(y)$, the Fourier transform of $g$, decays as $y^{-(d+1)}$ for large argument $y$. For large $q$, $Q(g) \approx p^2 U(g)$ where $U(g)$ is independent of $q$, and we define $\nu = \lim_{q\to\infty}\mu(q)\,p^2$. Then the eigenvalue problem can be solved exactly [12] with eigenfunction $g(x) = \operatorname{erfc}(x/\sqrt{2})$ and $\nu = 2(d-1)$. Thus, for large $q$, $\mu \sim 2(d-1)/p^2$, where $p^2 \approx \ln(q)$ and therefore $\lambda \approx d - (d-1)/\ln q$. We note that, for $d = 1$, a direct solution of Eq. (9) coincides with the exact solution of the $q$-state kinetic Potts model [12], with $g(x) = (1 - q^{-1})\operatorname{erf}(x) + q^{-1}$ and $\lambda = 1$.

We now compare our results with the direct $T = 0$ simulation of the $q$-state Potts model. We have also simulated directly our field theory [Eq. (3)] and found that it evolves in a similar way as the Potts model (see Ref. [12] for details), with domains growing as $L^2(t) \sim t$. The determination of $\lambda$ requires large lattices (especially for large $q$) and large numbers of Monte Carlo (MC) steps (typically $10^4$) which is easier to achieve in the Potts model simulation. The calculations have been carried out at $T = 0$ on an $800 \times 800$ square lattice with equal coupling to nearest and next nearest neighbors (NNN's). NNN interactions are needed at $T = 0$ to avoid pinning to the lattice for $q > 2$. It also ensures a better isotropy of surface tension, and thus of bubbles. We optimized the MC procedure by selecting only surface Potts spins for updating, since only these can be flipped at $T = 0$. For $q \leq 20$, the results for 20–40 samples were averaged, whereas 10–20 samples were found to be sufficient for $q > 20$, due to smaller fluctuations for $L(t)$ and $A(t)$ with increasing $q$, yielding, to our knowledge, the most extensive simulations to date. We find $L^2(t) \sim t$ for all $q$, and observe good scaling of the correlation function. In Table I, we present the values of $\lambda$ generated in simulations, and compare them to those obtained from the (numerical) solution of Eq. (9). We find a reasonably good agreement. We also note that $\lambda$ from the simulation saturates very slowly to its $q \to \infty$ value, as predicted by

TABLE 1. $\lambda$ for different $q$ as computed from the Potts model simulation and by solving the eigenvalue equation (9) numerically.

| $q$ | 2 | 10 | 20 | 30 | 50 | 100 | 200 | $+\infty$ |
|---|---|---|---|---|---|---|---|---|
| $\lambda_{\text{Potts}}$ | $1.25 \pm 0.01$ [a] | $1.40 \pm 0.02$ | $1.49 \pm 0.01$ | $1.57 \pm 0.01$ | $1.64 \pm 0.01$ | $1.72 \pm 0.01$ [c] | $1.82 \pm 0.02$ [c] | $1.99 \pm 0.01$ |
| $\lambda_{\text{theory}}$ | 1.289 [b] | 1.476 | 1.566 | 1.611 | 1.660 | 1.713 | 1.755 | 2.000 |

[a]See also Ref. [9].
[b]See also Ref. [11].
[c]For $q$ that large and the finite samples considered here, the effective $q$ is probably larger and $\lambda$ is slightly overestimated (see Ref. [12] for more details).

our asymptotic result. For $q = 2$, and in principle for other values of $q$ as well, $\lambda$ can be measured experimentally for systems with the Ising symmetry. For instance, the authors of Ref. [14] found $L(t) \sim t^{\phi}$, with $\phi = 0.515 \pm 0.026$ and $\lambda = 1.246 \pm 0.079$, compared to $\phi = \frac{1}{2}$ and $\lambda = 1.286\ldots$ in the Gaussian closure approximation [11], and $\lambda = 1.25 \pm 0.01$ numerically [9]. Mean-field or large $N$ approaches also give $\phi = \frac{1}{2}$, but lead to $\lambda = d$ and $\lambda = d/2$, respectively [12]. For soap bubbles, $q = \infty$ and $\lambda = 2$ ($\lambda = d$ in dimension $d$). Indeed, the choice $q = \infty$ eliminates the coalescence of bubbles with identical index, so that $A(t) \sim 1/N(t) \sim 1/L(t)^d$, where $N(t)$ is the number of remaining bubbles at time $t$. In Fig. 1, we compare the correlation function for $q \to \infty$ as given by the Potts model simulation, the direct simulation of the field theory for $q = 50$ fields on a $120 \times 120$ lattice, and by our approximate theory, and find good agreement. For soap bubbles, $g(x)$ measures the probability that the point $x$ belongs to the same bubble as the origin.

Finally, the correspondence between the correlation functions of the $q$-state Potts model and of the Ising model with a fixed average magnetization $\langle m_0 \rangle = 2/q - 1$ shows that $\lambda$ for the Ising model continuously depends on $\langle m_0 \rangle$, and may be close if not exactly equal to the value of $\lambda$ for the associated Potts model. This analogy also suggests a possible experimental observation of $\lambda$ and the correlation functions for $q > 2$, in magnetic bubbles [12,15].

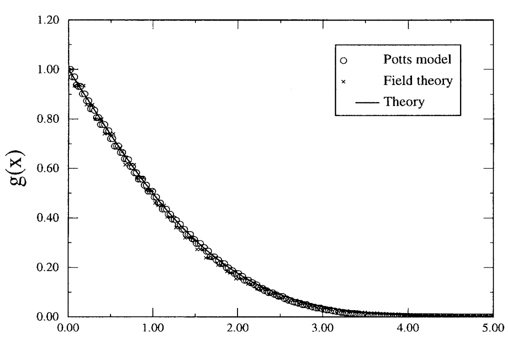


FIG. 1. Comparison of the scaled equal-time correlation functions generated by numerical simulation of the Potts model with $q = \infty$ (in fact $q$ equals the initial number of bubbles ~32 000), numerical integration of Eq. (3) with $q = 50$, and the large $q$ analytical result.

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