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Corrections to scaling in the q-state Potts model within Gaussian closure approximation

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Abstract. Corrections to scaling in the q-state Potts model due to departures of the initial condition from scaling morphology are studied at zero temperature in phase-ordering kinetics within Gaussian closure approximation. When the corrections to scaling are included, the equal time correlation function has the form $G(r,t) = g_0(r/L) + L^{-\omega} g_1(r/L) + \cdots$, where L is the coarsening length scale. Both the correction-to-scaling exponent ω and the correction-to-scaling function $g_1(x)$ are calculated for different values of q. The correction-to-scaling exponent ω is found to be nontrivial and depends on q. The corrections to scaling are found to be large (relative to scaling function $g_0(x)$ itself) at large scaling variable x.

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1 Introduction

There has been some considerable interest in phase ordering kinetics in the past few years [1]. When the system is quenched from a high temperature (disordered) phase into the two-phase or multi-phase regions, ordered phases grow as functions of time t. At later times, it is well established that when all length are scaled by the characteristic length scale $L(t) \sim t^n$, the system becomes time-independent. This means that quantities such as correlation function $G(r,t) = g(x)$, where $x = r/L$ is the scaling variable. For systems with short range correlations and two ordered phases, the growth exponent $n = 1/2$ for nonconserved (model A) dynamics, while $n = 1/3$ for locally conserved (model B) dynamics [1].

Apart from noncoserved and locally conserved dynamics, there has been some analytical, numerical and simulation studies [2–4] when the ordering of a system is subject to globally conserved dynamics. The dynamics of the order parameter in this case are the same as the model A dynamics subject to global conservation of the order parameter. It has been found that global conservation does not change the growth exponent $n = 1/2$. However, the autocorrelation function [5] and persistence exponent [6] were found to depend on whether the order parameter is globally conserved.

The phase ordering dynamics of a system which consists of more than two ordered phases such as q-state Potts model [7] have not been extensively studied [5]. It is well established that the growth exponent does not depend on the value of q but on the dynamics of a system. This means that $n = 1/2$ for the q-state Potts model undergoing nonconserved (and globally conserved) dynamics [5,8,9], while $n = 1/3$ for locally conserved dynamics [10]. It has been observed by Sire and Majumdar (SM) [5] that the evolution of $q = 2$ Potts model is equivalent to the evolution of an Ising model evolving with fixed magnetisation $m = 2/q - 1$. Other experimental realizations exist for $q = 3$, 4, ∞ [7]. The limit $q \to \infty$ correctly describes the coarsening phenomenon in metallic grains [9,11,12] and dry soap froth [13].

Calculations on corrections to scaling due to nonscaling initial condition for a number of models with both locally conserved and nonconserved dynamics have recently been done[14]. These corrections enters correlation function $G(r,t))$ as follows. $G(r,t) = g_0(r/L) + L^{-\omega} g_1(r/L) + \cdots$, where g_1 and ω are correction-to-scaling function and correction-to-scaling exponent respectively. Although, in most of the models studied ω was found to be trivial, for approximate calculations on realistic models ω was found to be nontrivial, dependent on dimensionality d of the system and the symmetry of the order parameter. The corrections to scaling were found to be more at large values of the scaling variable x.

This paper studies the corrections to scaling, associated with deviations of the order parameter from the scaling morphology in the initial state of the q-state Potts model within the Gaussian closure approximation [15]. We find that the correction-to-scaling exponent ω depends on

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q while the correction-scaling function $g_1(x)$ does not show strong dependence on q. In this paper we work within the thin domain wall limit [1] and for quenches to zero temperatures [1,16,17]. This leads to simplifications as corrections associated with domain wall thickness and thermal fluctuations are not considered.

The paper is organised as follows. In Section 2, q-state Potts model is discussed within field theory and Gaussian closure approximation, and some general concepts are introduced. Corrections to scaling are studied in Section 3. Section 4 concludes with a summary and discussion.

2 Field theory and Gaussian closure approximation

A "Gaussian closure" theory proposed by Mazenko [15] has been applied to q-state model by SM [5]. In the q-state Potts model, the two-point correlation function is defined as $G(12) = \sum_{l=1}^{q} \langle \phi_l(\mathbf{r}_1, t_1)\phi_l(\mathbf{r}_2, t_2)\rangle$. The angular brackets denote the average over initial conditions while "12" denotes the pair of space-time points $(\mathbf{r}_1, t_1)$ and $(\mathbf{r}_2, t_2)$. Applying the symmetry of the order parameter field $\phi(\mathbf{r}, t)$ and the translational invariance, the equal time correlation function becomes,

$$G(r,t) = q\langle \phi_l(\mathbf{r}_1, t)\phi_l(\mathbf{r}_2, t)\rangle, \tag{1}$$

where $r = |\mathbf{r}_2 - \mathbf{r}_1|$. The evolution equation for the equal time correlation function for q-state Potts model quenched to zero temperature is given by [5]

$$\frac{1}{2}\frac{\partial G(r,t)}{\partial t} = \nabla^2 G(r,t) - q \times \langle \phi_l(0,t)[V'(\phi_l(\mathbf{r},t)) - \langle\lambda_1\rangle]\rangle, \tag{2}$$

where $V(\phi)$ is the potential with q degenerate minima and λ_1 is the Lagrange's multiplier enforcing the constraint $\sum_l \phi_l = 1$.

The order parameter field $\phi(\mathbf{r}, t)$ varies sharply across the domain walls and as a result the evaluation of the last term in equation (2) has not yet been realised without approximations made. In order to evaluate the averages in the last two terms of equation (2), SM applied the Gaussian closure approximation developed by Mazenko [15]. Within the Gaussian closure approximation a nonlinear transformation is made from ϕ to a smooth varying auxiliary field $m(r,t)$. The nonlinear transformation $\phi(r,t) = \sigma[m(r,t)]$ is given by

$$\frac{d^2\sigma}{dm^2} + \frac{da}{dt}\frac{d\sigma}{dm} = V'(\sigma) - \langle\lambda_1\rangle, \tag{3}$$

where $a(t)$ accounts for moving frame [5] and is fixed by the condition that average on both sides of equation (3) must be the same. The assumption that the auxiliary field $m(r,t)$ has a Gaussian probability distribution enables the evaluation of the last term on the righthand side of equation (2) giving

$$\frac{1}{2}\frac{\partial G(r,t)}{\partial t} = \nabla^2 G(r,t) + \frac{1}{C_0(t)} f \frac{\partial G}{\partial f}, \tag{4}$$

where $f(r,t) = C(r,t)/C_0(t)$, is the normalised equal time correlation function of the auxiliary field $m(r,t)$,

$$C(r,t) = \langle\{m(\mathbf{r}_1, t) - \bar{m}(t)\}\{m(\mathbf{r}_2, t) - \bar{m}(t)\}\rangle \tag{5}$$

and

$$C_0(t) = \langle\{m(t) - \bar{m}(t)\}^2\rangle. \tag{6}$$

Note that $f(0,t) = 1$ and $f \to 0$ as $r \to \infty$. The relation between $f(r,t)$ and $G(r,t)$ has been explicitly given [5]

$$G(f) = \frac{q}{\sqrt{\pi}}\int_0^\infty \exp\left[-\left(y + p\sqrt{\frac{2}{1+f}}\right)^2\right] \times \operatorname{erf}\left[\sqrt{\frac{1+f}{1-f}}y\right] dy, \tag{7}$$

where $p = \operatorname{erfc}^{-1}[2/q]$. Note that $G(0,t) = 1$, and $G \to 1/q$ as $f \to 0$.

3 Corrections to scaling

3.1 The case q = 2

When $q = 2$ the last term in equation (4) can be easily expressed in terms of the correlation function $G(r,t)$ only. For $q = 2$, the correlation function $G(r,t)$ simplifies to

$$G(f) = \frac{2}{\pi}\arctan\left(\sqrt{\frac{1+f}{1-f}}\right). \tag{8}$$

The linear transformation $W(r,t) = 2G(r,t) - 1$ leads to the following boundary conditions: Both W and $G \to 1$ as $f \to 1$, while for $f \to 0$, $W \to 0$ and $G \to 1/2$. Since $0 \le f \le 1$, the linear transformation implies that $W(r,t) = 2/\pi \sin^{-1}(f)$. Using equation(4), it is straight forward to show that the evolution equation for W is given by

$$\frac{1}{2}\frac{\partial W(r,t)}{\partial t} = \nabla^2 W(r,t) + \frac{1}{C_0(t)}\frac{1}{\pi}\tan\left(\frac{\pi}{2}W(r,t)\right). \tag{9}$$

The above equation is similar to Mazenko result [15] and the corrections to scaling in this case were obtained in our previous work [14]. The results will be included in Table 1 for completeness.

3.2 The case when q > 2

For $q > 2$, $f(r,t)$ cannot be eliminated from equation (4) in favor of $G(r,t)$ and as a result we will work with $f(r,t)$ instead of $G(r,t)$. From dimensional analysis $C_0(t) \sim L^2$ and is chosen [5] as $C_0(t) = L^2/\mu$, where μ is a constant to be determined by physical arguments [15]. Expressing equation (4) in terms of $f(r,t)$ leads to

$$\frac{1}{2}\frac{\partial f}{\partial t} = \frac{G_{ff}}{G_f}\left(\frac{\partial f}{\partial r}\right)^2 + \frac{\partial^2 f}{\partial r^2} + \frac{d-1}{r}\frac{\partial f}{\partial r} + \frac{\mu}{L^2}f, \tag{10}$$

where $G_f = dG/df$ etc. Corrections to scaling can be imposed on $f(r,t)$ since $G(r,t)$ is a function of $f(r,t)$. In the scaling limit, $G(r,t)$ approaches the scaling function $g_0(r/L)$ which is L-independent if all lengths are scaled by L and $L\frac{dL}{dt}$ is constant as $L \sim t^{1/2}$. Including corrections to scaling due to nonscaling scaling initial condition in the usual way [14] leads to

$$\begin{aligned} f(r,t) &= f_0\left(\frac{r}{L}\right) + L^{-\omega} f_1\left(\frac{r}{L}\right) + \cdots, \\ G(r,t) &= g_0\left(\frac{r}{L}\right) + L^{-\omega} g_1\left(\frac{r}{L}\right) + \cdots, \\ \frac{dL}{dt} &= \frac{2}{L} + \frac{b}{L^{1+\omega}} + \cdots, \end{aligned} \tag{11}$$

where

$$\begin{aligned} g_0\left(\frac{r}{L}\right) &= G(f_0), \\ g_1\left(\frac{r}{L}\right) &= f_1\left(\frac{r}{L}\right)\left[\frac{dG}{df}\right]_{f=f_0}, \end{aligned} \tag{12}$$

and b is a constant.

Using equations (11) in (10), and equating leading and next-to-leading powers of L leads to

$$f_0'' + \frac{G_{f_0 f_0}}{G_{f_0}} f_0'^2 + \left[x + \frac{d-1}{x}\right] f_0' + \mu f_0 = 0 \tag{13}$$

and

$$\begin{aligned} f_1'' &+ \left[x + \frac{d-1}{x}\right] f_1' + [\mu + \omega]\, f_1 \\ &+ \frac{b}{2} x f_0' + 2\frac{G_{f_0 f_0}}{G_{f_0}} f_0' f_1' \\ &+ \left[\frac{G_{f_0 f_0 f_0}}{G_{f_0}} - \frac{(G_{f_0 f_0})^2}{{G_{f_0}}^2}\right] f_1 f_0'^2 = 0. \end{aligned} \tag{14}$$

The primes indicate derivatives with respect to the scaling variable $x = r/L$ and $G_{f_0} = [dG/df]_{f=f_0}$, etc.

Both equations (13) and (14) cannot be solved analytically. However, they can be integrated numerically subject to the appropriate initial conditions imposed at $x = 0$. At $x = 0$, $f_0 = 1$. The initial conditions can be obtained by letting $f_0 \to 1$. In this limit

$$G(f) \approx 1 - p\sqrt{\frac{2}{\pi}}\ (1-f)^{1/2}, \tag{15}$$

from which G_f, etc, can easily be found. In the small-x limit, the scaling and correction-to-scaling function are given by

$$f_0 = 1 - \frac{\mu}{2(d-1)}x^2 + \cdots \tag{16}$$

and

$$f_1 = \frac{\mu}{4(d^2-1)}x^4 + \cdots \tag{17}$$

respectively.

Table 1. The autocorrelation exponent λ and the correction-to-scaling exponent ω for different values of q in $d = 2$ and $d = 3$.

	$d=2$		$d=3$	
q	λ	ω	λ	ω
2	1.289	3.884	1.673	3.903
10	1.476	3.991	1.946	4.020
100	1.713	4.292	2.397	4.491
200	1.755	4.333	2.485	4.610

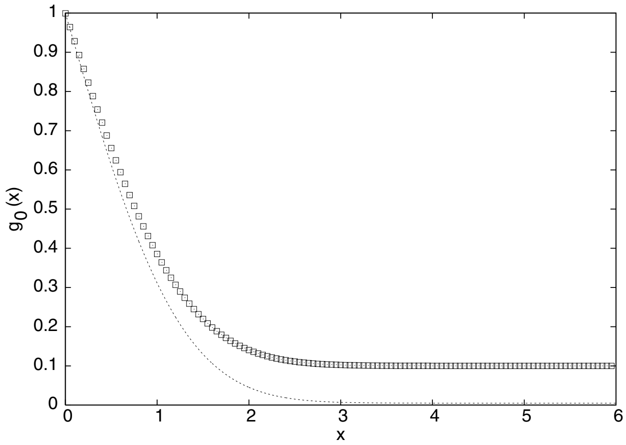

Fig. 1. The scaling function $g_0(x)$ in $2d$. The boxed and broken lines correspond to $q = 10$ and $q = 200$ respectively.

In the large-x limit $f_0 \to 0$, while $G \to 1/q$ and as a result equation (13) can be linearised as the second term becomes negligible. There are two linearly independent solutions with asymptotic forms $f_{01} \sim x^{-\mu}$ and $f_{02} \sim x^{\mu-d}\exp(-x^2/2)$ as $x \to \infty$. The amplitudes of both solutions depends on μ, in order to solve equation (13), μ is chosen in such a way that the power law solution is absent since the system has short range correlations [5,15]. Note that μ is related to autocorrelation exponent λ via $\lambda = d - \mu/2$. Values of λ for different values of q are given in Table 1. The values of λ are in reasonable agreement with simulations [5] and experiments [18].

For equation (14), there are two linearly independent solutions in the large-x limit. One with a power-law tail

$$f_{11} \sim x^{-(\omega+\mu)} \tag{18}$$

and the other with a Gaussian tail

$$f_{12} \sim x^{v}\exp(-x^2/2), \tag{19}$$

where $v = \mu - d + \omega$ if $\omega > 2$ and $v = \mu - d + 2$ otherwise. The correction-to-scaling exponent ω is determined by the condition that the power-law decaying term is absent from the large-x solution. Implementing this condition numerically gives values of ω for different values of q in $d = 2$ and $d = 3$. The values of ω are shown in Table 1.

Having determined the solutions of equation (13) and equation (14), we use these results to find the scaling function $g_0(x)$ and the correction-to-scaling function $g_1(x)$ from equations (7) and (12). Figure 1 shows scaling function $g_0(x)$ while Figure 2 shows the correction-to-scaling

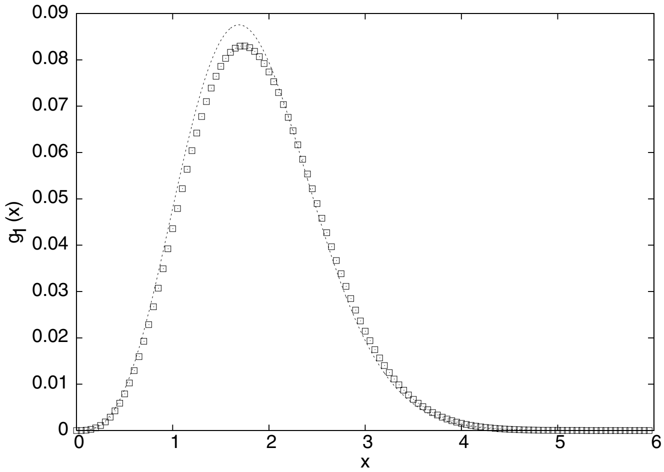

Fig. 2. The correction-to-scaling function $g_1(x)$ in $2d$. The boxed and broken lines correspond to $q = 10$ and $q = 200$ respectively.

function $g_1(x)$, in $2d$ for $q = 10$ and 200. The scaling function $g_0(x)$ shows strong dependence on q especially in the large-x limit, as $g_0(x) \to 1/q$ in this limit. The correction-to-scaling function $g_1(x)$ shows no strong dependence on q. The amplitude of $g_1(x)$ is fixed by the constant b in equation (14). The value $b = 2$ was used in Figure 2.

Now we consider the case $d \to \infty$ for $q = 2$. Including corrections to scaling in equation (9), we let

$$\begin{aligned} W(r,t) &= h_0\left(\frac{r}{L}\right) + L^{-\omega} h_1\left(\frac{r}{L}\right) + \cdots, \\ \frac{dL}{dt} &= \frac{2}{L} + \frac{b}{L^{1+\omega}} + \cdots, \end{aligned} \tag{20}$$

where $h_0(x)$ is the scaling function and $h_1(x)$ is the correction to-scaling function. Note that the actual correlation function $G(r,t)$ is related to the function $W(r,t)$ via the relation

$$W(r,t) = 2G(r,t) - 1. \tag{21}$$

Substituting equations (20) in (9) and retaining the leading and the next leading powers of L^ω leads to

$$h_0'' + \left(\frac{d-1}{x} + x\right) h_0' + \frac{\mu}{2\pi} \tan\left(\frac{\pi}{2} h_0\right) = 0 \tag{22}$$

$$h_1'' + \left(\frac{d-1}{x} + x\right) h_1' + \mu \sec^2\left(\frac{\pi}{2} h_0\right) h_1 + \omega h_1 + \frac{b}{2} x h_0' = 0. \tag{23}$$

For large-d, from equation (22) it is clear that $\mu \propto d$ in order to cancel the term dh_0'/x. Retaining only this term, the exact solution (with initial condition $h(0) = 1$) is

$$h_0(x) = \frac{2}{\pi} \sin^{-1}\left(\exp[-x^2/2]\right), \tag{24}$$

with $\mu = d$. The condition that $h_0(x) \sim \exp(-x^2/2)$ for large-x has also been used.

The corrections to scaling can be found by large-x analysis of equation (23). For large-x, the term $\sec^2(\pi h_0/2) \to 1$ and equation (23) reduces to the correction-to-scaling equation

$$h_1'' + \left(\frac{d-1}{x} + x\right) h_1' + \mu h_1 + \omega h_1 + \frac{b}{2} x h_0' = 0. \tag{25}$$

The solution to the above equation is given by

$$\begin{aligned} h_1(x) &= \frac{bx^4}{2(4d+8)} \exp\left(-\frac{x^2}{2}\right), \\ \omega &= 4. \end{aligned} \tag{26}$$

The above analysis shows that in the limit $d \to \infty$ for $q = 2$; $\mu = d$ and $\omega = 4$ while the scaling function

$$G_0(x) = \frac{1 + \frac{2}{\pi} \sin^{-1}\left(\exp[-x^2/2]\right)}{2}, \tag{27}$$

and the correction-to-scaling function

$$G_1(x) = \frac{bx^4}{4(4d+8)} \exp\left(-\frac{x^2}{2}\right). \tag{28}$$

However, it is not clear at present how the same analysis employed above for $d \to \infty$ can be extended to $q > 2$. This is due to the complicated dependence of the correlation function $G(r,t)$ on f and q for $q > 2$.

4 Summary

Corrections to scaling due to nonscaling initial condition have been studied for q-state Potts model within the Gaussian closure approximation. The correction-to-scaling function $g_1(x)$ and the associated correction-to-scaling exponent ω, have been calculated for different values of q in 2 and $3d$. We have found that ω, in general is a nontrivial exponent, which depends on q and d, and increases as q increases. We have as yet been unable to find ω and $g_1(x)$ analytically in the limit of large q. This remains an interesting open question, especially because $q \to \infty$ correctly describes the evolution of a dry soap froth [13] and the growth of metallic grains [9,11,12]. The analytical calculations in this limit would also help in determining the limiting values of ω (if any) as q increases. It is worth mentioning that analytical solution for the scaling function $g_0(x)$ has been realised by looking at the limit $g_0(x) \to 1$ [5], in this limit the correction-to-scaling function $g_1(x)$ vanishes.

The corrections to scaling are relatively small (compared to the scaling function itself) at small-x. This implies that when comparing simulation or experimental data with theory, small-x region must be given more weight as the corrections to scaling are small.

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