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Scaling exponent β for coarsening in a 1D q-state system

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Abstract. An exponent β which characterises non-equilibrium coarsening processes is calculated in a deterministic solvable model of coarsening for a 1D q-state system. We study how the fraction of sites P which have never changed their state, scale with the characteristic domain length $\langle\ell\rangle$. β is defined by $P \sim \langle\ell\rangle^{\beta-1}$. We propose a new model of coarsening that prevents correlations from developing between domains thereby ensuring tractability and an exact result for any q.

1. Introduction

Domain coarsening occurs when a system is rapidly quenched from a high-temperature disordered state to a low-temperature ordered state [1]. Domains of different equilibrium ordered states form and grow with time. In an infinite system this competition between different ordered domains goes on forever and the system thus remains far from equilibrium at all times. The study of this time-dependent morphology of the growing domains has been of major interest for the past few decades [1]. An important observation towards characterizing these patterns is that they exhibit dynamic scaling at late times. This means the domain structure at later times is statistically similar to those at earlier times except for a global change of a single length scale [1]. This implies that at late times the system is characterized by a *single* length scale $\langle\ell(t)\rangle$ and all time-dependent quantities exhibit scaling in terms of this $\langle\ell(t)\rangle$. The scaling hypothesis implies that the equal-time and two-time correlation function can be written in scaling form as

$$C(r,t) = f(r/\langle\ell\rangle) \qquad C(r,t,t') = (\langle\ell\rangle'/\langle\ell\rangle)^{\lambda} h(r/\langle\ell\rangle).$$

These scaling forms are well supported by experiment [1].

It is believed that the exponents and scaling functions of a phase ordering system is controlled by the $T = 0$ strong-coupling fixed point. This means that thermal noise is irrelevant for late time scaling properties and it is sufficient to study the coarsening only at $T = 0$. Theoretically there have been two main approaches to study the zero-temperature coarsening process [1]. The first is to study discrete stochastic spin models such as the Ising or Potts model evolving via Glauber dynamics [2] and the second is to study deterministic models such as the noiseless Ginzburg–Landau (GL) equation for the coarse-grained order parameter. In this case the GL equations are completely deterministic, the only randomness being in the initial conditions. This is very different from the kinetic Ising models, which are stochastic by definition (even at $T = 0$) and the average of any thermodynamic quantity is not only over initial conditions (which is the case for the $T = 0$ GL equations) but also over

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the evolution histories. It is generally believed that in $d \geqslant 2$ the stochastic and deterministic models belong to the same universality class, but in 1D the situation is quite different [4]. For example, for the 1D Ising model, with Glauber dynamics, at $T = 0$, evolved from a random initial condition (quenching from high T), the domain walls perform independent random walks and annihilate upon meeting. The average domain size $\langle \ell \rangle$ grows as $t^{1/2}$. The equal-time and the two-time spin–spin correlation functions can be exactly calculated [2, 3]. On the other hand for deterministic models the situation is different. For example, in the 1D GL model the domain walls interact via their exponential tails leading to a logarithmic growth law [4]. This kind of a difference in time dependence suggests that exponents defined with respect to $\langle \ell \rangle$ may be more fundamental than those defined with respect to t.

The correlation function exponents and the dependence of the characteristic domain length scale on time have been studied extensively [1–4]. However, since this gives no information on the history of evolution of the system, the study of 'persistence' is important. A simple way of characterizing the history of evolution of a system would be to look at, say, the probability of a single spin in an Ising system not changing its spin up to a certain time, in other words, its 'persistence' in clinging to its original state. By studying the scaling behaviour with $\langle \ell \rangle$ of P, the fraction of spins that have not changed their state, we can define the exponent β by $P \sim \langle \ell \rangle^{\beta - 1}$. For the stochastic 1D Ising model with Glauber dynamics an exact result for β was found [5] to be $\beta = 0.25$. The same exponent was studied in the context of the 1D GL model whose late time dynamics can be mapped, as will be explained later, to a deterministic coarsening algorithm which consists of the continual removal of the smallest domains. In this case it was found [6] to be exactly $0.824\ldots$.

The same question can be asked in the context of the q-state Potts model. It turns out that though the autocorrelation exponent and the growth law for the characteristic domain length may be the same, β varies with q. An exact result [5] was recently found for the 1D stochastic case, which is an exact generalization of the $q = 2$ case, as

$$\beta(q) = \frac{5}{4} - \frac{4}{\pi^2}\left[\cos^{-1}\left(\frac{2-q}{\sqrt{2}q}\right)\right]^2 .$$

Noting the difference between the value of β in the stochastic and deterministic cases for $q = 2$, it is only natural to ask how β for the deterministic case differs from its stochastic counterpart for general q. However, for $q > 2$ deterministic models, correlations develop between neighbouring domains as opposed to the $q = 2$ case [6]. This makes it difficult to solve the deterministic case exactly for $q > 2$. Nevertheless, approximate solutions have been obtained by ignoring these correlations [7, 8]. In this paper, we present a modified version of the deterministic model in which no correlations develop between domains which makes it exactly solvable. Our exact calculation shows that the exponent β depends continuously on q. Our model reduces to the true deterministic model for $q = 2$ but not for higher values of q.

2. The model

The motivation behind our model is as follows. Let us consider the $q = 2$ Ising case first, in the context of the time-dependent GL equation in 1D with no noise ($T = 0$). It turns out [9, 4] that the late time dynamics of this model can be mapped to deterministic equations describing the motions of a set of interacting domain walls (kinks in the wall profile). The kinks interact via an exponential attractive interaction. This implies that in the limit when the typical separation between domain walls is much larger than the width of a wall, the shortest domains collapse instantly as compared with the longer ones. This means that the dynamics reduces to a deterministic model where at each timestep the shortest domain is found and the spins inside it are flipped. Thus the system coarsens with the continual 'removal' of the shortest domains.

Now we can address the question as to what fraction of the spins have never flipped. It is clear that once a domain has been removed the spins inside no longer contribute to the fraction of spins that have never flipped. If we call those parts of the line where the spins have flipped at least once 'wet', and those parts where the spins have never flipped 'dry', then clearly, when a domain is removed, the portion of the line it occupied becomes 'wet'. So the question about the scaling of the fraction of spins that have never flipped can be rephrased as: how does the density of dry regions scale with $\langle \ell \rangle$? We define the exponent β by saying that the dry region density scales as $\langle \ell \rangle^{\beta-1}$ or the dry part per domain goes as $\langle \ell \rangle^{\beta}$.

A straightforward generalization of this procedure to the q-state Potts model can be made. The domains form a random sequence constructed from the q available states, no two consecutive domains being the same. Again the smallest domains will collapse and can be removed if the states of the domains on either side are the *same*, but if they are *different* the two walls will coalesce to form a new wall at the midpoint. However, this routine leads to correlations developing between the domains. Instead we consider a model in which the smallest domain is merged with the domain to its right if the states of the domains on either side are different. This ensures, as we shall shortly explain, that no correlations develop between domains. This leads to tractability and an exact result for any q. In this paper we examine how the dry region density scales with the characteristic domain length scale in the context of this model.

At any time we have a sequence of domains constructed from the q available states, no two consecutive ones being the same. The smallest domains are identified at each timestep. If the domains to its left and right are the in the *same* state then it flips to *that* state, that is, the three domains merge to form a single large domain. Since domains remain uncorrelated, as we shall show, the probability of this occurence is $\frac{1}{q-1}$. On the other hand with a probability $\frac{q-2}{q-1}$ (in the event that the two domains are in different states), the smallest domain flips to the state of its right-hand neighbour. In other words, it merges with its right-hand neighbour leaving the other neighbour unaffected. In both cases the part of the line previously occupied by the smallest domain becomes wet.

Now we consider the question of correlations. Suppose we choose N intervals, the number of distinct arrangements of these on a circle is $(N-1)!$. Suppose we deterministically coarsen this system by picking the smallest domain each time and removing it, till we end up with one interval. Thus $(N-1)!$ distinct histories can be created. Now we consider an alternate algorithm which consists of picking the smallest interval and then picking two intervals at random and combining the three. We iterate this procedure until only a single interval remains. This procedure also generates $(N-1)!$ histories which are in one-to-one correspondence with the histories generated by the deterministic algorithm described above. This proves that no correlations develop between domains during coarsening by merging with domains to *both* the left and right.

Now consider coarsening the N intervals arranged on a circle by picking the smallest interval each time and combining it with the interval to the right. This procedure generates $(N-1)!$ histories. As before we consider an alternative procedure of picking the smallest interval at each step and picking another interval at random and attatching it to the smallest interval. This procedure also generates $(N-1)!$ histories again proving that the coarsening algorithm does not develop any correlations between the domains.

So we have proved that the coarsening procedure we use in our model, which is nothing but a combination of the two coarsening algorithms described above, does not allow correlations to develop between intervals. As a result we can use the 'picking at random' algorithm to compute β.

3. Equation for β

Our calculations follow the method used by Bray *et al* [6] for the 1D Ising model case. We start with random intervals on a line. Each interval I is characterized by its length $l(I)$ and by the length of its dry part $d(I)$. At each timestep the smallest domain $I_{\min}$ is picked. As explained before there are two possibilities.

(1). Two more intervals I_1, I_2 are picked at random. The three domains are merged to form a single large domain I. This occurs with probability $\frac{1}{q-1}$. The total length and dry parts of I are given by

$$l(I) = l(I_1) + l(I_{\min}) + l(I_2) \tag{1}$$

$$d(I) = d(I_1) + d(I_2). \tag{2}$$

(2). Another interval I_1 is picked at random. The smallest domain is merged with it to form a new domain I. This occurs with probability $\frac{q-2}{q-1}$. The length and dry part of I are given by

$$l(I) = l(I_1) + l(I_{\min}) \tag{3}$$

$$d(I) = d(I_1). \tag{4}$$

We assume that the lengths of intervals take only integer values and that the minimal length in the system is i_0. We also assume that there is a very large number N of intervals. We denote the number of intervals of length i by n_i and also the average length of the dry part of intervals of length i by d_i. We denote by primed symbols the values of these quantities after all the n_{i_0} intervals of length i_0 have been eliminated, so that the minimal length becomes $i_0 + 1$. The time evolution equations are then given by

$$N' = N - 2n_{i_0}\left(\frac{1}{q-1}\right) - n_{i_0}\left(\frac{q-2}{q-1}\right) \tag{5}$$

i.e.

$$N' = N - n_{i_0}\left(\frac{q}{q-1}\right). \tag{6}$$

Similarly we have

$$n'_i = n_i\left(1 - \left(\frac{q}{q-1}\right)\frac{n_{i_0}}{N}\right) + \frac{n_{i_0}}{q-1}\sum_{j=i_0}^{i-2i_0}\frac{n_j}{N}\frac{n_{i-j-i_0}}{N} + \frac{q-2}{q-1}n_{i_0}\left(\frac{n_{i-i_0}}{N}\right) \tag{7}$$

$$\begin{aligned} n'_i d'_i = n_i d_i\left(1 - \left(\frac{q}{q-1}\right)\frac{n_{i_0}}{N}\right) + \frac{n_{i_0}}{q-1}\sum_{j=i_0}^{i-2i_0}\frac{n_j}{N}\frac{n_{i-j-i_0}}{N}(d_j + d_{i-j-i_0}) \\ + \left(\frac{q-2}{q-1}\right)\frac{n_{i_0}}{N}(n_{i-i_0}d_{i-i_0}). \end{aligned} \tag{8}$$

Note that these are valid for $n_{i_0} \ll N$ which is valid when i_0 becomes large. We assume that after many iterations i.e. when i_0 becomes large, a scaling regime is reached, where

$$n_i = \frac{N}{i_0}f\left(\frac{i}{i_0}\right) \qquad n_i d_i = N i_0^{\beta-1} g\left(\frac{i}{i_0}\right). \tag{9}$$

For large i_0 we can treat $x = i/i_0$ as a continuous variable. Then neglecting $O(1/i_0^2)$ we have

$$n'_i = \frac{N'}{i_0+1} f\left(\frac{i}{i_0+1}\right) = \frac{N}{i_0}\left[f(x) - \left(\frac{q}{q-1}\right)\frac{f(1)}{i_0}f(x) - \frac{f(x)}{i_0} - x\frac{f'(x)}{i_0}\right] \tag{10}$$

and

$$\begin{aligned} n'_i d'_i &= N'(i_0+1)^{\beta-1} g\left(\frac{i}{i_0+1}\right) \\ &= N i_0^{\beta-1}\left[g(x) - \left(\frac{q}{q-1}\right)\frac{f(1)}{i_0}g(x) + \frac{\beta-1}{i_0}g(x) - x\frac{g'(x)}{i_0}\right]. \end{aligned} \tag{11}$$

Inserting these into the time evolution equations (7) and (8), and using the fact that f and g are independent of i_0 for large i_0 we obtain

$$\begin{aligned} &f(x) + xf'(x) + \theta(x-3)\frac{f(1)}{q-1}\int_1^{x-2} f(y)f(x-y-1)\,\mathrm{d}y \\ &\qquad + \theta(x-2)\left(\frac{q-2}{q-1}\right)f(1)f(x-1) = 0 \end{aligned} \tag{12}$$

$$\begin{aligned} &(1-\beta)g(x) + xg'(x) + 2\theta(x-3)\frac{f(1)}{q-1}\int_1^{x-2} g(y)f(x-y-1)\,\mathrm{d}y \\ &\qquad + \theta(x-2)\left(\frac{q-2}{q-1}\right)f(1)g(x-1) = 0. \end{aligned} \tag{13}$$

Now we introduce the Laplace tranforms of the functions f and g

$$\phi(p) = \int_1^\infty \exp(-px)f(x)\,\mathrm{d}x \tag{14}$$

$$\psi(p) = \int_1^\infty \exp(-px)g(x)\,\mathrm{d}x. \tag{15}$$

Taking Laplace transforms of equations (12) and (13) we obtain

$$p\phi'(p) = f(1)\exp(-p)\left[\left(\frac{1}{q-1}\right)\phi^2(p) + \left(\frac{q-2}{q-1}\right)\phi(p) - 1\right] \tag{16}$$

$$p\psi'(p) + \beta\psi(p) = f(1)\exp(-p)\left[2\left(\frac{1}{q-1}\right)\psi(p)\phi(p) + \left(\frac{q-2}{q-1}\right)\psi(p) - \frac{g(1)}{f(1)}\right]. \tag{17}$$

These are fairly simple first-order differential equations in one variable and may be solved in a straightforward fashion to obtain the solutions

$$\phi(p) = \frac{1-\exp(-h(p))}{1+\left(\frac{1}{q-1}\right)\exp(-h(p))} \tag{18}$$

$$\psi(p) = g(1)\int_p^\infty \left[\frac{1+\frac{1}{q-1}\exp(-h(x))}{1+\frac{1}{q-1}\exp(-h(p))}\right]^2 \frac{\exp(h(x))}{\exp(h(p))}\frac{x^{\beta-1}}{p^\beta}\exp(-x)\,\mathrm{d}x \tag{19}$$

where $h(x)$ is given by

$$h(x) = f(1)\left(\frac{q}{q-1}\right)\int_x^\infty \frac{\mathrm{e}^{-t}}{t}\,\mathrm{d}t. \tag{20}$$

It may be noted that the constants of integration implied by the form of the solutions above, are fixed by the requirement that both ϕ and ψ go to zero as p tends to infinity.

It remains to fix the constants $f(1)$ and β. For this we use the following expansion

$$\int_p^\infty \frac{\mathrm{e}^{-x}}{x}\,\mathrm{d}x = -\ln(p) - \gamma - \sum_{n=1}^{\infty}\frac{(-p)^n}{nn!} \tag{21}$$

where γ is Euler's constant and has a value $\gamma = 0.577\,215\ldots$. Using this with (18) and (20) gives a small p expansion for ϕ

$$\phi(p) = 1 - \left(1 + \frac{1}{q-1}\right) p^{\frac{q}{q-1}f(1)} \exp\left[\frac{q}{q-1} f(1)\gamma\right](1 + \mathrm{O}(p)). \tag{22}$$

Comparing this with the small p expansion from (14) which is $\phi(p) = 1 - \langle x\rangle p + \cdots$ we obtain $f(1) = \frac{q-1}{q}$ and also the ratio of the mean domain length to the minimum length as $\langle x\rangle = \left(\frac{q}{q-1}\right)\mathrm{e}^{\gamma}$.

The exponent β can be determined in a similar fashion. We define $r(p)$ by

$$r(p) = h(p) + \ln(p) = -\gamma - \sum_{n=1}^{\infty}\frac{(-p)^n}{nn!}. \tag{23}$$

Using this we can rewrite (19) as

$$\psi(p) = g(1)\int_p^\infty \left[\frac{1 + \frac{x}{q-1}\exp(-r(x))}{1 + \frac{p}{q-1}\exp(-r(p))}\right]^2 \frac{\exp(r(x))}{\exp(r(p))}\frac{x^{\beta-2}}{p^{\beta-1}}\exp(-x)\,\mathrm{d}x. \tag{24}$$

From this we may obtain the small p form of $\psi(p)$ as

$$\frac{g(1)}{1-\beta} + \frac{g(1)}{1-\beta}\mathrm{e}^{\gamma} p^{1-\beta} B(p,\beta) \tag{25}$$

where

$$B(p,\beta) = \int_p^\infty x^{\beta-1}\frac{\mathrm{d}}{\mathrm{d}x}\left[\mathrm{e}^{-x}\left(\mathrm{e}^{\frac{r(x)}{2}} + \frac{1}{q-1}x\mathrm{e}^{\frac{-r(x)}{2}}\right)^2\right]\mathrm{d}x. \tag{26}$$

It may be easily shown that

$$B(p,\beta) = B(0,\beta) + \mathrm{O}(p^{1+\beta}) + \mathrm{O}(p^{2+\beta}) + \cdots. \tag{27}$$

Thus (25) reduces to

$$\frac{g(1)}{1-\beta}(1 + B(0,\beta)p^{1-\beta} + \mathrm{O}(p) + \mathrm{O}(p^2) + \cdots). \tag{28}$$

We now compare this expansion to the direct expansion of $\psi(p)$ obtained from (15), namely $\psi(p) = \int_1^\infty \mathrm{d}x\, g(x)(1 - p(x) + \mathrm{O}(p^2))$. If we require the function $g(x)$ to have a finite first moment then we must have $B(0,\beta) = 0$ i.e

$$\int_0^\infty x^{\beta-1}\frac{\mathrm{d}}{\mathrm{d}x}\left[\mathrm{e}^{-x}\left(\mathrm{e}^{\frac{r(x)}{2}} + \frac{1}{q-1}x\mathrm{e}^{\frac{-r(x)}{2}}\right)^2\right]\mathrm{d}x = 0. \tag{29}$$

This condition determines β for us. For general q the β can be determined by numerical methods from the above condition (29). We have computed β for sample values of q (see table 1). We have computed β for q = 2 that agrees with Bray's value [6] up to the five decimal places. This is what one would expect because, as we mentioned before, our model reduces to Bray's model for $q = 2$. We also notice a monotonic decrease in β as q increases (see figure 1). This is also what one would physically expect if we look at the dry part *per domain* which scales as $\langle\ell\rangle^{\beta}$. As we go to higher values of q, coarsening proceeds almost exclusively by the smallest domain merging with *one* nearest neighbour. This implies that,

Table 1. β for various q.

q	β
2	0.824 92. . .
3	0.680 92. . .
4	0.581 78. . .
5	0.509 40. . .
7	0.409 99. . .
10	0.319 05. . .
50	0.083 21. . .

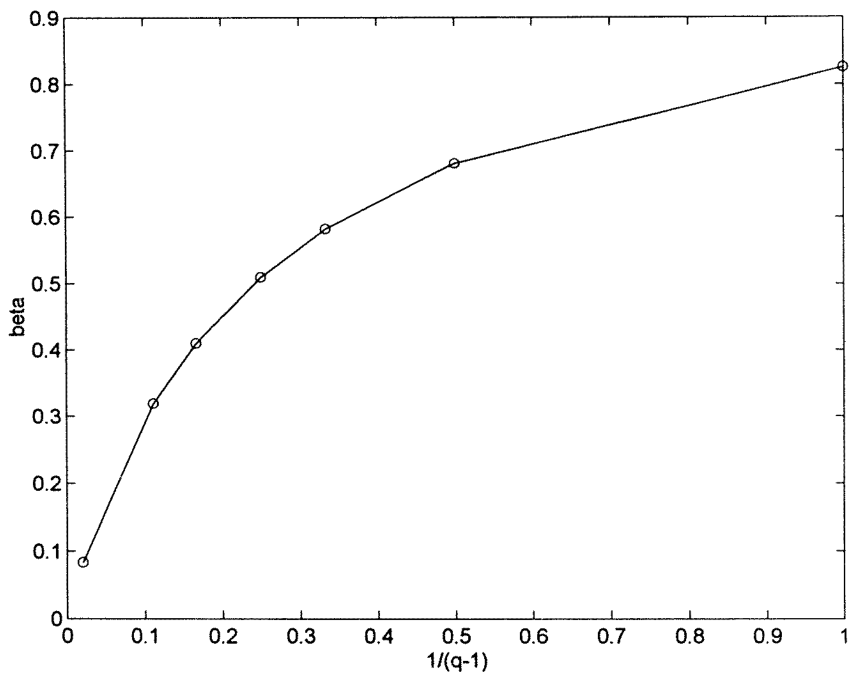

Figure 1.

in the scaling regime, the dry part per domain remains almost *constant* leading to lower and lower values of β, which indeed, is what we find. It can also be shown analytically by considering the small p form of $\psi(p)$ for the $q \to \infty$ case that $\beta = 0$.

4. Conclusion

We have studied a deterministic model of coarsening for the zero-temperature dynamics of a q-state system in 1D. This model does not allow correlations to develop between domains thus rendering it exactly solvable. We have determined the persistence exponent β exactly for all q. For $q = 2$, we obtain $\beta = 0.824\ldots$ in complete agreement with [6]. As q increases we find that the exponent β decreases monotonically to 0.

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