Scaling Exponent for Coarsening in a 1D q-state system.

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Abstract

An exponent \( \beta \) which characterises non-equilibrium coarsening processes is calculated in a deterministic solvable model of coarsening for a 1D q-state Potts system. We study how the fraction of sites \( P \) which have never changed their state, scale with the characteristic domain length \( \langle \ell \rangle \). \( \beta \) 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 \( q \).

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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 states form on larger and larger length scales

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Thus giving us a system that is forever in nonequilibrium. An important observation is that this nonequilibrium coarsening process exhibits dynamic scaling at late times, that is, the domain structure at later times is statistically similar to those at earlier times except for a global change of scale [1]. This implies that at late times the system is characterized by a single length scale \( \ell(t) \) and all properties of the system can be got in terms of this \( \ell(t) \). The scaling hypothesis implies that the equal time and two time correlation function can be written in scaling form as

\[
C(r, t) = f\left(\frac{r}{\langle \ell \rangle}\right) \quad C(r, t, t') = \left(\frac{\langle \ell \rangle'}{\langle \ell \rangle}\right)^h\left(\frac{r}{\langle \ell \rangle}\right)
\]

These scaling forms are well supported by experiment.

Theoretically there have been two main approaches to studying the coarsening process. The first is to study stochastic models such as the Ising model with Glauber dynamics and the second is to study deterministic models like the Ginzburg-Landau equation for the coarse grained order parameter with no noise term. 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 the histories of evolution. It is generally believed that in \( d \geq 2 \) the stochastic and deterministic models belong to the same universality class. But in 1D the situation is quite different. 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 behave as independent random walkers who 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 [1,2,3,4].
But 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 $\beta$ by $P \sim \langle \ell \rangle^{\beta-1}$. For the stochastic 1D Ising model with Glauber dynamics an exact result for $\beta$ 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...

The same question can be asked in the context of the q-state Pott’s model. It turns out that though the autocorrelation exponent and the growth law for the characteristic domain length may be the same, $\beta$ 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

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

Noting the difference in value of $\beta$ in the stochastic and deterministic case for $q = 2$, it is only natural to ask how $\beta$ varies for general $q$ in the deterministic case. For general $q$, however tractability is lost because, as we shall explain later, correlations develop between domains. Nevertheless approximate calculations ignoring these correlations have been carried out [7,8].

In this paper we present a different model of coarsening in which no correlations develop between domains. Using this model we can calculate $\beta$ exactly for any $q$. For $q = 2$ our model reduces to the case discussed above.

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 Ginzburg-Landau equation in 1D with no noise ( \( T = 0 \) ). It turns out \([4]\) 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 to the longer ones. This means that the dynamics reduces to a deterministic model where at each time step 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 \( \beta \) 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 Pott’s model can be done. 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. But this routine leads to correlations developing between the domains. Instead we consider an abstract 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 abstract model.
The details of the model are as follow.

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 time step. If the domains to its left and right are 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 occurrence 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 side 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 attaching 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 $\beta$.

3. Equation for $\beta$

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 characterised by its length $l(I)$ and by the length of its dry part $d(I)$. At each time step the smallest domain $I_{\text{min}}$ 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

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

$$d(I) = d(I_1) + d(I_2)$$

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

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

$$d(I) = d(I_1)$$

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

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

Similarly we have

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

\[ n'_i d'_i = n_i d_i \left( 1 - \left( \frac{q}{q-1} \right) \frac{n_{i_0}}{N} \right) + \frac{n_{i_0}}{q-1} \sum_{j=i_0}^{i-2i_0} \frac{n_j}{N} \frac{n_{i-j-i_0}}{N} (d_j + d_{i-j-i_0}) + \left( \frac{q-2}{q-1} \right) \frac{n_{i_0}}{N} \left( n_{i-i_0} d_{i-i_0} \right) \]  

Note that these are valid for \( n_{i_0} << N \) 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

\[ n_i = \frac{N}{i_0} f \left( \frac{i}{i_0} \right) \]  
\[ n_i d_i = N i_0^{\beta-1} g \left( \frac{i}{i_0} \right) \]  

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

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

and

\[ n'_i d'_i = N(i_0 + 1)^{\beta-1} g \left( \frac{i}{i_0+1} \right) \]

\[ = N i_0^{\beta-1} \left[ g(x) - \left( \frac{q}{q-1} \right) \frac{f(1)}{i_0} g(x) + \frac{\beta-1}{i_0} g(x) - x \frac{g'(x)}{i_0} \right] \]
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 get

\[
f(x) + xf'(x) + \theta(x - 3) \frac{f(1)}{q - 1} \int_1^{x-2} f(y) f(x - y - 1) dy
\]

\[
+ \theta(x - 2) \left( \frac{q-2}{q-1} \right) f(1) f(x - 1) = 0
\] (12)

\[
(1 - \beta)g(x) + xg'(x) + 2\theta(x - 3) \frac{f(1)}{q - 1} \int_1^{x-2} g(y) f(x - y - 1) dy
\]

\[
+ \theta(x - 2) \left( \frac{q-1}{q-2} \right) f(1) g(x - 1) = 0
\] (13)

Now we introduce the Laplace tranforms of the functions \( f \) and \( g \)

\[
\phi(p) = \int_1^\infty \exp(-px) f(x) dx
\] (14)

\[
\psi(p) = \int_1^\infty \exp(-px) g(x) dx
\] (15)

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

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

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

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

\[
\phi(p) = \frac{1 - \exp(-h(p))}{1 + \left( \frac{1}{q-1} \right) \exp(-h(p))}
\] (18)
\[ \psi(p) = g(1) \int_p^\infty \left[ \frac{1 + \frac{1}{q-1} \exp(-h(x))}{1 + \frac{1}{q-1} \exp(-h(p))} \right]^2 \frac{\exp(h(x)) x^{\beta-1}}{\exp(h(p)) p^{\beta-1}} \exp(-x) \, dx \]  
\tag{19} \]

where \( h(x) \) is given by

\[ h(x) = f(1) \left( \frac{q}{q-1} \right) \int_x^\infty \frac{e^{-t}}{t} \, dt \]  
\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 \( \phi \) and \( \psi \) go to zero as \( p \) tends to infinity.

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

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

where \( \gamma \) is Euler’s constant and has a value \( \gamma \approx 0.577215 \). Using this with (18) and (20) gives a small \( p \) expansion for \( \phi \)

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

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

The exponent \( \beta \) 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

\[ \psi(p) = g(1) \int_p^\infty \left[ \frac{1 + \frac{1}{q-1} \exp(-r(x))}{1 + \frac{1}{q-1} \exp(-r(p))} \right]^2 \frac{\exp(r(x)) x^{\beta-2}}{\exp(r(p)) p^{\beta-1}} \exp(-x) \, dx \]  
\tag{24} \]
From this we may get the small $p$ form of $\psi(p)$ as

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

(25)

where

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

(26)

It may be easily shown that

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

(27)

Thus (25) reduces to

$$\frac{g(1)}{1 - \beta} \left( 1 + B(0, \beta)p^{1 - \beta} + O(p) + O(p^2) + ... \right)$$

(28)

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

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

(29)

This condition determines $\beta$ for us. For general $q$ the $\beta$ can be determined by numerical methods from the above condition (29). We have computed $\beta$ for sample values of $q$ (see table). $\beta$ for $q = 2$ agrees with Bray’s value [6] upto the 5 decimal places we have computed. 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 $\beta$ as $q$ increases. 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, in the scaling regime, the dry part per domain remains almost constant leading to lower and lower values of $\beta$, 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 Pott’s system in 1D following a rapid quench. This model does not allow correlations to develop between domains thus rendering it exactly solvable. We have determined the persistence exponent $\beta$ exactly for all q. For $q = 2$ we obtain $\beta = 0.824...$ in complete agreement with [6]. As q increases we find that $\beta$ decays monotonically to zero.
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Table 1: $\beta$ for various $q$

| $q$ | $\beta$          |
|-----|------------------|
| 2   | 0.82492...       |
| 3   | 0.68092...       |
| 4   | 0.58178...       |
| 5   | 0.50940...       |
| 7   | 0.40999...       |
| 10  | 0.31905...       |
| 50  | 0.08321...       |