Coarsening in the 1D Ising model evolving with Swendsen - Wang dynamics: an unusual scaling

1996 J. Phys. A: Math. Gen. 29 L589

(http://iopscience.iop.org/0305-4470/29/23/002)

J. Phys. A: Math. Gen. **29** (1996) L589–L594. Printed in the UK

LETTER TO THE EDITOR

Coarsening in the 1D Ising model evolving with Swendsen–Wang dynamics: an unusual scaling

Bernard Derrida†‡ and Vincent Hakim†

† Laboratoire de Physique Statistique, ENS, 24 rue Lhomond, 75005 Paris, France
‡ Service de Physique Théorique, CE Saclay, F91191 Gif sur Yvette, France

Received 10 September 1996

Abstract. We consider a simple model of domain growth: the zero-temperature 1D Ising model evolving according to the Swendsen–Wang dynamics. We find that in the long-time limit, the pair correlation function scales with a characteristic length increasing as the square of the average domain size. In that limit, a few large domains occupy almost all the space with many small domains between them. In contrast to the usual picture of coarsening, the average domain size here is not a characteristic length of the growth problem. Instead, one finds a power-law distribution for the sizes of large domains with a cut-off at a length which grows as the square of the average size of the domains.

Coarsening phenomena in two-phase systems, like Ising models below their ordering temperature, have attracted a lot of interest in the last decades [1, 2]. The usual picture is that, in the long-time limit, there is a scaling regime with a single characteristic length, the average size λ of the domains (usually, this average size grows as a power law with time $\lambda \sim t^{\alpha}$). However, a two-length scaling has been found in some systems [3, 4].

The goal of the present work is to describe a simple example of coarsening in a two-phase system which also exhibits an unusual scaling with a characteristic length Λ much larger than the average domain size λ and a power-law distribution for the size of large domains with a cut-off at Λ.

The system we consider is the zero-temperature Ising chain evolving according to a Swendsen–Wang-like dynamics [5, 6]: during every infinitesimal time interval Δt, each spin has a probability Δt of being updated and updating a spin means that the whole cluster containing this spin is flipped. In other words, each domain I (of length $l(I)$) has a probability $\Delta t \; l(I)$ of flipping during the infinitesimal time interval Δt. (The flipping interval I means that three intervals, itself and its right and left neighbours, I_1 and I_2, are replaced by a single interval of length $l(I) + l(I_1) + l(I_2)$).

Clearly, during each time interval Δt, the total number $N(t)$ of domains (which is also the number of frustrated bonds) decreases (on average) by $2L\Delta t$ (where L is the total length of the system), so that as long as $N(t)$ is very large, its expression is given by

$$N(t) = N(0) - 2Lt$$

If at time $t = 0$, there is a density $\rho_0 = N(0)/L$ of domains, the density at time t becomes

$$\rho = \rho_0 - 2t$$

0305-4470/96/230589+06$19.50

and the whole system is reduced to a single domain when $t \to \rho_0/2$. The average domain size λ which is

$$\lambda = \frac{L}{N(t)} = \frac{1}{\rho_0 - 2t}$$

diverges as $t \to \rho_0/2$. We are interested in the regime where the average domain size λ becomes very large, but is still much smaller than the system size L in order to have a large number of domains in the system and to avoid the late stage of the growth where some domains become comparable in size to the total system size L (this late stage regime would be dominated by fluctuations as the sizes of the largest domains in this regime would fluctuate from sample to sample). Mathematically, this means that here we want to take the limit $L \to \infty$ first and then the limit $t \to \rho_0/2$. For simplicity in what follows, we will mostly consider two cases for the initial condition: randomly oriented spins (case I) and an antiferromagnetic initial condition (case II).

The reason which makes possible the calculation of the distribution of domain sizes is that one can write an exact evolution equation for this distribution. If one defines $N_i(t)$ the number of intervals of length i, the evolution of the total number of intervals $N(t)$

$$N(t) = \sum_i N_i(t)$$

and of the $N_i(t)$ is given by

$$N(t + \Delta t) = N(t) - 2L\Delta t$$

$$N_i(t + \Delta t) = N_i(t) + \Delta t \left[-iN_i(t) - 2L\frac{N_i(t)}{N(t)} + \sum_j \sum_k jN_j(t)\frac{N_k(t)}{N(t)}\frac{N_{i-j-k}(t)}{N(t)} \right]. \tag{1}$$

Equation (1), which *a priori* looks like a mean-field equation is in fact exact for the following two reasons. First, because if initially the lengths of the intervals along the line are not correlated (as in cases I and II), they remain uncorrelated at any later time. This is because whenever an interval is updated, it merges with its two nearest neighbours but does not acquire any correlation with its remaining neighbours and so the process preserves the absence of correlations [7]. The second reason which makes (1) valid is that we consider a system in the limit $L \to \infty$. Therefore all the $N_i(t)$ are self-averaging quantities.

Clearly the process keeps the total length L constant:

$$L = \sum_i iN_i(t)$$

As $L \to \infty$, it is more convenient to work with the densities

$$\rho(t) = \frac{N(t)}{L} \qquad \rho_i(t) = \frac{N_i(t)}{L}$$

(for randomly oriented spins (case I) $\rho(0) \equiv \rho_0 = \frac{1}{2}$ and $\rho_i(0) = 2^{-i-1}$, whereas for an antiferromagnetic initial condition (case II) $\rho(0) \equiv \rho_0 = 1$ and $\rho_i(0) = \delta_{i,1}$). These densities evolve according to (1):

$$\frac{\mathrm{d}\rho_i(t)}{\mathrm{d}t} = -i\rho_i(t) - 2\frac{\rho_i(t)}{\rho(t)} + \sum_j \sum_k \frac{j\rho_j(t)\ \rho_k(t)\ \rho_{i-j-k}(t)}{\rho^2(t)} \tag{2}$$

and as

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -2 \tag{3}$$

one can consider the $\rho_i(t)$ as functions of $\rho(t)$ and rewrite (2) as

$$2\frac{d\rho_i}{d\rho} = i\rho_i + 2\frac{\rho_i}{\rho} - \sum_j \sum_k \frac{j\rho_j\ \rho_k\ \rho_{i-j-k}}{\rho^2}. \tag{4}$$

Equation (4) is valid when $L \to \infty$, and the long-time regime we want to consider is the limit of large domains ($\rho \to 0$). It has the form of a Smoluchowski equation [8] in a case where gelation occurs at a finite time ($= \rho_0/2$).

By multiplying (4) by i^n and by summing over n it is easy to generate evolution equations for the moments σ_n defined by

$$\sigma_n = \sum_i \rho_i\ i^n.$$

In addition to the known fact that

$$\sigma_0 = \rho \qquad \text{and} \qquad \sigma_1 = 1$$

this gives the following evolution equations:

$$\frac{\mathrm{d}\sigma_2}{\mathrm{d}\rho} = -\frac{2\sigma_2}{\rho} - \frac{1}{\rho^2}$$

$$\frac{\mathrm{d}\sigma_3}{\mathrm{d}\rho} = -\frac{3\sigma_3}{\rho} - \frac{3\sigma_2^2}{\rho} - \frac{6\sigma_2}{\rho^2}$$

$$\frac{\mathrm{d}\sigma_4}{\mathrm{d}\rho} = -\frac{4\sigma_4}{\rho} - \frac{10\sigma_2\sigma_3}{\rho} - \frac{10\sigma_3}{\rho^2} - \frac{15\sigma_2^2}{\rho^2}$$

and so on. The evolution equation of σ_n involves only σ_n itself or lower moments, and so in principle the whole hierarchy can be solved:

$$\begin{aligned}\sigma_2 &= \frac{B}{\rho^2} - \frac{1}{\rho}\\ \sigma_3 &= \frac{3B^2}{\rho^4} + \frac{C}{\rho^3} + \frac{3}{\rho^2}\\ \sigma_4 &= \frac{15B^3}{\rho^6} + \frac{10BC + 15B^2}{\rho^5} + \frac{D}{\rho^4} - \frac{15}{\rho^3}\end{aligned} \tag{5}$$

etc, where the integration constants $B, C, D, \ldots$ depend only on the initial condition. The above expressions of the first moments indicate that for $n \geqslant 1$ and $\rho \to 0$

$$\sigma_n \sim \left(\frac{B}{\rho^2}\right)^{n-1}$$

meaning that the intervals which contribute mostly to the moments have a length of order ρ^{-2} whereas the average size of the domains is of order ρ^{-1}.

An easy way of obtaining all the moments σ_n is to consider the generating function

$$g(s) = \sum_i \mathrm{e}^{si}\ \rho_i = \sum_n \frac{s^n}{n!}\sigma_n \tag{6}$$

From (4), one can easily derive the evolution equation of $g(s)$:

$$\frac{\partial g}{\partial \rho} = \frac{1}{2}\frac{\partial g}{\partial s} + \frac{g}{\rho} - \frac{g^2}{2\rho^2}\frac{\partial g}{\partial s} \tag{7}$$

and so given an initial distribution of domain sizes and its generating function $g_0(s)$, one can follow $g(s)$ as $\rho \to 0$ by integrating (7). For example, if initially the spins are random (case I), one has $\rho_i = 2^{-i-1}$ and this implies $\rho = \frac{1}{2}$ and $g_0(s) = \mathrm{e}^s/(2 - \mathrm{e}^s)$ for the initial condition, whereas if the initial configuration is antiferromagnetic (case II), $\rho_i = \delta_{i,1}$ and $g_0(s) = \mathrm{e}^s$ for $\rho = 1$.

In principle (7) can be solved exactly by the method of characteristics. It is convenient to introduce the function h such that $g(s) = \rho h(s)$, as neither ρ nor s appear explicitly in the equation that h satisfies:

$$\frac{\partial h}{\partial \rho} = \frac{1}{2}\frac{\partial h}{\partial s} - \frac{h^2}{2}\frac{\partial h}{\partial s}.$$

For example, in case I, one can show that $h(s)$ is solution of

$$2s + (1 - h^2)\left(\rho - \frac{1}{2}\right) - 2\log\frac{2h}{h+1} = 0 \tag{8}$$

whereas in case II, it is given by the solution of

$$2s + (1 - h^2)(\rho - 1) - 2\log h = 0. \tag{9}$$

More generally, if in the initial condition the density is ρ_0 and the function h is $h_0(s)$, the solution $h(s)$ is given implicitly in terms of s and ρ by the solution of

$$h_0\left(s + \tfrac{1}{2}(1 - h^2)(\rho - \rho_0)\right) = h. \tag{10}$$

The solution is in general complicated enough to make the explicit expression of the ρ_i difficult to obtain in the limit $\rho \to 0$.

As for $\rho \to 0$ one expects from (5) that all integer moments $\sigma_n \sim (B/\rho^2)^{n-1}$ (except $\sigma_0 = \rho$), the generating function $g(s)$ should satisfy the following scaling:

$$g(s) - \rho \simeq \frac{\rho^2}{B} G\left(\frac{Bs}{\rho^2}\right) \tag{11}$$

where according to (5), $G(0) = 0$, $G'(0) = 1$, $G''(0) = 1$, $G^{(3)}(0) = 3$ and $G^{(4)}(0) = 15$. If one tries to find a solution of the form (11), one obtains the requirement that $G(x)$ should satisfy the following equation:

$$G - 2xG' + GG' = -\frac{\rho}{2B}G^2G' - \rho\frac{\partial G}{\partial \rho} \tag{12}$$

where $x = Bs/\rho^2$. In the long-time limit, $\rho \to 0$ and one finds that the following expression for $G(x)$:

$$G(x) = 1 - \sqrt{1 - 2x} \tag{13}$$

becomes a solution of (12) satisfying $G'(0) = 1$.

The constant B can be obtained from the initial condition $B = \sigma_2\rho^2 + \rho$. For randomly oriented spins in the initial condition (case I), one has $\rho = \frac{1}{2}$ and $\sigma_2 = 3$ so that $B = \frac{5}{4}$. For an antiferromagnetic initial configuration (case II), $\rho = 1$, $\sigma_2 = 1$ and $B = 2$. This agrees with (8)–(10) when one looks for a solution $g(s) = \rho h(s)$ in the limit $\rho \to 0$ and $s \sim \rho^2$ and one uses the fact that $h_0(s) = 1 + s/\rho_0 + (B - \rho_0)s^2/2\rho_0^3 + \mathrm{O}(s^3)$ as (10) becomes $s - \rho(h-1) + B(h-1)^2/2 = 0$. The solution of this quadratic equation recovers (11) and (13).

From (11), (13), one can see that for all $n \geqslant 1$

$$\sigma_n \simeq \frac{\Gamma(n - \frac{1}{2})}{\sqrt{\pi}}\left(\frac{2B}{\rho^2}\right)^{n-1}$$

and if one defines a length Λ by

$$\Lambda = 2B/\rho^2$$

for $i \sim \Lambda$ one has

$$\rho_i \simeq \frac{1}{\sqrt{\pi}} \frac{1}{\Lambda^{1/2}} \frac{1}{i^{3/2}} \mathrm{e}^{-i/\Lambda} \tag{14}$$

It is interesting to note that the long-time behaviour of all the integer moments is determined by the knowledge of ρ and σ_2 in the initial condition, i.e. by the first two moments of the initial distribution of the lengths of the intervals.

Expression (14) does not hold down to $i \sim 1$. For $i \sim 1$, the ρ_i have more complicated expressions than (14) and all the details of the initial distribution of domain sizes become important, even in the limit $\rho \to 0$. For example, if the initial spin configuration is random (case I) one can calculate easily the ρ-dependence of the first ρ_i from (4), and one finds

$$\rho_1 = \tfrac{1}{2}\rho\mathrm{e}^{(2\rho-1)/4} \qquad \rho_2 = \tfrac{1}{4}\rho\mathrm{e}^{(2\rho-1)/2} \qquad \rho_3 = \tfrac{1}{32}(5\rho - 2\rho^2)\mathrm{e}^{(6\rho-3)/4}$$

whereas for an initial antiferromagnetic configuration (case II), one finds

$$\rho_1 = \rho\mathrm{e}^{(\rho-1)/2} \qquad \rho_2 = 0 \qquad \rho_3 = \tfrac{1}{2}(\rho - \rho^2)\mathrm{e}^{(3\rho-3)/2}.$$

These two examples show that as $\rho \to 0$, a finite fraction of domains are domains of length 1 (with $\rho_1 \simeq \rho\mathrm{e}^{-1/4}/2$ in case I and $\rho_1 \simeq \rho\mathrm{e}^{-1/2}$ in case II). Clearly the spins belonging to these domains of length 1 are spins which never flipped under the dynamics. So the picture is that in the limit $\rho \to 0$, almost all the line is occupied by large domains of size of order $\Lambda \sim \rho^{-2}$ whereas almost all domains are small of size of order 1. Between two consecutive large domains, there are an infinite number of small domains.

This picture can be confirmed by calculating the pair correlation function $\langle S_0 S_R \rangle$ between two spins at positions 0 and R. Because the sizes of successive domains are uncorrelated it is possible to relate the distribution of domain sizes and the correlation function [9, 10]. This relation is easier to write for the Laplace transforms. If

$$F(s) = \sum_{R \geqslant 0} \mathrm{e}^{sR} \langle S_0 S_R \rangle$$

one can show in a very similar way to [9, 10] that

$$F(s) = 2\rho \, \frac{\mathrm{e}^s}{(\mathrm{e}^s - 1)^2} \, \frac{g(s) - \rho}{g(s) + \rho} - \frac{1}{\mathrm{e}^s - 1}$$

which, using (11), in the limit $\rho \to 0$ and $s \sim \rho^2$ becomes

$$F(s) \sim \frac{1}{s} \left[\frac{\rho^2}{Bs} G\left(\frac{Bs}{\rho^2} \right) - 1 \right]. \tag{15}$$

It is easy to check that the same expression would be obtained in this limit ($\rho \to 0$, $s \sim \rho^2$) if $\langle S_0 S_R \rangle$ was given only by the contribution of the pairs belonging to the same domain, i.e.

$$\langle S_0 S_R \rangle_{\mathrm{approx}} \simeq \sum_{i \geqslant R} (i - R)\rho_i$$

as this would give

$$F_{\mathrm{approx}}(s) = \frac{\mathrm{e}^s}{(\mathrm{e}^s - 1)^2} \, (g(s) - \rho) - \frac{1}{\mathrm{e}^s - 1}$$

which becomes identical to (15) when $\rho \to 0$ and $s \sim \rho^2$. This is because between two large domains, there are always so many small domains that the contributions of an even or an odd number of these small domains almost cancel.

From (14) it follows that when $\rho \to 0$, $\langle S_0 S_R \rangle$ becomes a function of the ratio $x = R/\Lambda$:

$$\langle S_0 S_R \rangle \simeq \sum_{i \geqslant R} \frac{1}{\sqrt{\pi}} \frac{1}{\Lambda^{1/2}} \frac{i-R}{i^{3/2}} \mathrm{e}^{-i/\Lambda} \simeq \int_x^\infty \frac{\mathrm{d}y}{\sqrt{\pi}} \; \frac{y-x}{y^{3/2}} \; \mathrm{e}^{-y}.$$

Note that for $x \to 0$, $\langle S_0 S_R \rangle \simeq 1 - 4x^{1/2}/\sqrt{\pi}$. The limit 1 as $x \to 0$ means that domains described by (14), i.e. of size $\sim \Lambda$, occupy almost all the space (as two spins at a distance small compared with Λ are likely to be parallel). The fact that the correction is $x^{1/2}$ means that between two such large domains, there are infinitly many small domains in contrast to normal cases [2], where the first correction is linear in x.

Another quantity one can consider is the fraction r of persistent spins [7, 11] (the spins which never flip up to time t). As all the spins belonging to domains of length 1 have never flipped, one has $r \geqslant \rho_1 \sim \rho$. One does not expect a large contribution from large domains as most of the spins of large domains have flipped many times. We did a simulation which confirmed that $r \sim \rho$ when $\rho \to 0$. This, in fact, can be shown analytically but we omit the details here, because the calculation of the limiting value of the ratio r/ρ as $\rho \to 0$ is rather complicated.

The calculations done above in the Ising case can be easily generalized to the Potts model. For Potts spins, each domain carries one of q colours and each time a domain is updated, all the spins of this domain adopt the colour of one of the two neighbouring domains (chosen at random). Therefore, if initially the spins are randomly chosen, when a domain is updated, it merges with its two neighbours with probability $1/(q-1)$, with its left neighbour only with probability $(q-2)/(2q-2)$ and with its right neighbour only with probability $(q-2)/(2q-2)$. This means that for general q and if the initial condition is random ($\mathrm{d}\rho/\mathrm{d}t = -q/(q-1)$), the mean-field-like equation (4) becomes

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}\rho} = \frac{q-1}{q} i\rho_i + \frac{\rho_i}{\rho} - \frac{q-2}{q} \sum_j \frac{j\rho_j \;\; \rho_{i-j}}{\rho} - \frac{1}{q} \sum_j \sum_k \frac{j\rho_j \;\; \rho_k \;\; \rho_{i-j-k}}{\rho^2} \qquad (16)$$

In contrast to other dynamical rules [7], this equation is still exact for arbitrary q, as the dynamics preserve the absence of correlation between the lengths of the domains. As $\rho \to 0$ the solution takes also the scaling form (11) except that

$$\sigma_2 = B/\rho^2 - 2/q\rho$$

with $B = (q+3)(q-1)/q^2$ (as $\rho_0 = (q-1)/q$ and $\sigma_2 = (q+1)/(q-1)$ for random initial conditions). So up to a change of the constant B, the picture in the Potts case is the same as in the Ising case.

References

[1] Langer J 1992 *Solids Far From Equilibrium* ed C Godrèche (Cambridge: Cambridge University Press)
[2] Bray A J 1994 *Adv. Phys.* **43** 357
[3] Coniglio A and Zannetti M 1989 *Europhys. Lett.* **10** 575
[4] Frachebourg L, Krapivsky P L and Ben-Naim E 1996 *Phys. Rev. Lett.* **77** 2125
[5] Swendsen R H and Wang J S 1987 *Phys. Rev. Lett.* **58** 86
[6] Wolff U 1989 *Phys. Rev. Lett.* **62** 361
[7] Bray A J, Derrida B and Godrèche C 1994 *Europhys. Lett.* **27** 175–80
[8] Van Dongen P G J and Ernst M H 1987 *J. Stat. Phys.* **49** 879
[9] Majumdar S N, Sire C, Bray A J and Cornell S J 1996 *Phys. Rev. Lett.* **77** 2867
[10] Derrida B, Hakim V and Zeitak R 1996 *Phys. Rev. Lett.* **77** 2871
[11] Derrida B, Hakim V and Pasquier V 1995 *Phys. Rev. Lett.* **75** 751–4