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Coarsening and percolation in the Ising Model with quenched disorder

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Abstract. Through large-scale numerical simulations, we study the phase ordering kinetics of the $2d$ Ising Model after a zero-temperature quench from a high-temperature homogeneous initial condition. Analysing the behaviour of two important quantities – the winding angle and the pair-connectedness – we reveal the presence of a percolating structure in the pattern of domains. We focus on the pure case and on the random field and random bond Ising Model.

1. Introduction

Phase ordering kinetics, the ordering of a system via domain growth after a quench from the homogeneous phase into one with broken symmetry, has attracted great interest in the last 50 years [1].

A simple example is a ferromagnet, instantaneously cooled (quenched) from above to below the critical point. The initial equilibrium state becomes unstable after the quench and evolves towards one of the two possible symmetry-related ordered configurations with opposite magnetizations. Relaxation toward the new equilibrium state occurs slowly (i.e. not exponentially fast) by the formation and growth (coarsening) of domains of the two equilibrium phases (i.e. group of aligned spins). This domain growth is driven by superficial tension, i.e. the interfaces tend to become flatter due to energetic reasons. Over time, the smallest domains disappear so that the typical size $R(t)$ of the remaining ones increases.

One theoretical approach to this class of problem is the kinetic Ising Model (IM), originally introduced by Glauber [2]. One starts with a Ising system in which each spins is randomly oriented, a situation that can be described as equilibrium at infinite temperature, $T \rightarrow \infty$. Then, the evolution of the system is treated as a Markov chain, with appropriate transition probabilities. The dynamical evolution can be simulated through standard Monte Carlo methods [3]. In the thermodynamic limit, the coarsening process goes on indefinitely, with none of the two equilibrium phases (up and down spins in this case) prevailing at any given finite time. This means that the magnetic system does not develop a magnetization, or equivalently that on average up spins are in the same number as down spins.



It was recently shown [4, 5, 6] that, after a transient from the quench, some of the morphological features of the coarsening domains in an ordinary, homogeneous IM are the same as those of a geometrical lattice at the percolation threshold p_c of random site percolation [7]. In such condition, a spanning (percolating) cluster is present. In the coarsening IM, we observe a percolating domain of either up or down spins. This fact may seem paradoxical, since percolation is a non-interacting problem, whereas coarsening is driven by spin-spin interactions. Moreover, the absence of magnetization in the coarsening system means that the percolative structures are present when 1/2 of spins are up (down). For a $2d$ square lattice, the same geometry we will consider for the IM, the critical percolation threshold is $p_c \simeq 0.59$, when occupying sites randomly. This means that we observe percolation in the coarsening IM when the occupation probability of up (down) spins is $1/2 < p_c$. This is not a contradiction, however, since after the transient t_p , the spin configuration is no longer random, having been shaped by the spin-spin interactions. It is, indeed, only after the coarsening dynamics has gone on for a transient that percolative features appear, while they are absent right after the quench, a sign that they are due to interactions. This can be phrased by saying that the spin-spin interactions lower the percolation threshold from $p_c \simeq 0.59$ to $1/2$. Moreover, although random uncorrelated percolation and correlated coarsening coexist on the same lattice, they live on separate length scales: the percolative properties are not present, at any given time, on length scales that are smaller than $R(t)$, the typical size of the domains, i.e. the correlated regions.

In a recent work [8], we showed that this phenomenology is also found in two types of inhomogeneous IM, where structural (quenched) disorder is present. In particular, we focussed on the random field Ising Model (RFIM) and random bond Ising Model (RBIM).

In this paper, after a brief review of the models considered and of the Monte Carlo algorithm implemented (Sec. 2), we define the relevant observables in Sec. 3 and present the basic results which highlight the occurrence of the percolation transition in Sec. 4.

2. Models and algorithm

We consider a $2d$ square lattice of linear size L , and the Hamiltonian of our models is

$$\mathcal{H}(\{S_i\}) = - \sum_{\langle ij \rangle} J_{ij} S_i S_j + \sum_i H_i S_i, \quad (1)$$

where S_i are the Ising variables and $\langle ij \rangle$ are two nearest-neighboring sites. The different models considered in our study are determined by the properties of the coupling constant J_{ij} and of the external field H_i , as follows.

Homogeneous IM: In this case, $H_i \equiv 0$ and $J_{ij} \equiv J_0$, i.e. we recover the ordinary IM. We also refer to it as the clean or pure model.

RFIM: The couplings are constant $J_{ij} \equiv J_0$, while the external fields H_i are drawn from a symmetric bimodal distribution and uncorrelated in space, i.e. $H_i = \pm h$, each with probability one half. We refer to this model as the RFIM.

RBIM: No external field, $H_i \equiv 0$, while the couplings are $J_{ij} = J_0 + \delta_{ij}$, where δ_{ij} are independent random numbers drawn from a uniform distribution in $[-\delta, +\delta]$. We keep $\delta < J_0$ in order to avoid frustration effects. We refer to this model as the RBIM.

In the case of the RBIM, coarsening via domain growth still takes place in the absence of frustration, which is the case we have considered. In the case of the RFIM, the Imry-Ma argument [9] tells us that ordering takes place up to a length

$$\ell_{IM} \sim \left(\frac{h}{J_0} \right)^{\frac{2}{d-2}}. \quad (2)$$

As we will see below, we focus on the case in which $\ell_{IM} \rightarrow \infty$, for which the system orders in any dimension.

As mentioned above, we can treat the dynamical evolution of the system as a Markov chain and simulate it through the Metropolis algorithm. Specifically, our algorithm flips single spins with Glauber transition rate

$$w(S_i \rightarrow -S_i) = \frac{1}{2} \left[1 - S_i \tanh \left(\frac{H_i^W + H_i}{T} \right) \right], \quad (3)$$

where the Weiss Field H_i^W , is given by

$$H_i^W = \sum_{j \in nn(i)} J_{ij} S_j, \quad (4)$$

with j running over the nearest-neighbors of the spin S_i .

For our simulations, the protocol consists in preparing a system of uncorrelated spins with no magnetization – equilibrium at $T \rightarrow \infty$ – and letting it evolve through single-spin flip according to Eq. (3). Performing the quench to T_f amounts to inserting the value of T_f into Eq. (3). We have let $T_f \rightarrow 0$ keeping the ratios $\epsilon = \frac{\delta}{T_f}$ (for RBIM) and $\epsilon = \frac{h}{T_f}$ (for RFIM) finite.

First, let us notice that this limit entails $\ell_{IM} \rightarrow \infty$, as mentioned above. Moreover, this simplifies the form of the transition rates, which depend only on the parameter ϵ . Not only we obtain a theory that depends on a single parameter, but simulations are sped up and thermal noise is reduced. More details on this algorithm and on its reliability can be found in [10, 11].

3. Key observables

The first quantity we consider, an essential one for the study of the phase ordering kinetics of a system, is the typical domain size $R(t)$. This is also referred to as *growing length*, since it grows while the system orders through domain growth. We have computed it as the inverse of the density of defects, i.e. dividing the number of couple of unaligned spins by L^2 . As discussed in [12], this is a standard method to estimate $R(t)$. We have then performed, as for all other quantities, an ensemble average, typically on $10^5 - 10^6$ realizations. $R(t)$ grows as $t^{1/2}$ in the pure system and slower and slower for increasing values of the parameter ϵ controlling the strength of disorder. More details can be found in [13].

In order to probe the emergence of percolation in the coarsening process, we used two observables : the average squared winding angle and the pair-connectedness function. They are naturally defined on a geometrical lattice in which a fraction p of the sites is occupied. They can be measured on an Ising lattice by identifying occupied sites as, say, up spins and empty sites as down spins, or vice-versa. A domain can then be considered as a cluster of up (or down) spins and the above quantities can be computed with respect to the domains of the system.

The (average squared) winding angle is defined considering the external contours – hulls – of a cluster of occupied sites. One considers two points P and Q at a distance x along the hull, and the tangent to the hull in these two points. The angle between the two tangents, measured counterclockwise in radians units, is the winding angle $\theta(P, Q)$. By fixing x , one can calculate the average winding angle for two points separated by this distance, $\langle \theta(x) \rangle$. It can be exactly proven, through methods of conformal field theory, that on a lattice at the percolation threshold for the hull of any cluster we have [14, 15]

$$\langle \theta^2(r) \rangle = a + \frac{4k}{8+k} \ln r, \quad (5)$$

where a is a constant and $k = 6$. This equation holds when $r \gg r_0$, r_0 being the lattice spacing, i.e. when the microscopic structure of the lattice can be ignored. Therefore, we will report

numerical data only for the largest domain of the system, so to have the largest possible range in which $r \gg r_0$.

The pair-connectedness function is defined in percolation theory as the probability that two occupied sites at distance r belong to the same cluster. From $2d$ percolation theory, we know that at $p = p_c$ [16, 17]

$$C_{perc}(r, r_0) \sim \left(\frac{r}{r_0}\right)^{-2\Delta} \quad (6)$$

where r_0 is the unit of length, usually the lattice spacing. Eq. (6) holds for $r \gg r_0$, with the critical exponent $\Delta = 5/48$. In the coarsening system we measure the pair-connectedness at any given time, identifying all the domains of up and down spins and then computing

$$C(r, t) = \frac{1}{4L^2} \sum_i \sum_{i_r} \langle \delta_{S_i, S_{i_r}} \rangle, \quad (7)$$

where $\delta_{S_i, S_j} = 1$ if the two spins belong to the same domain – namely they are aligned and there is a path of aligned spins connecting them – and $\delta_{S_i, S_j} = 0$ otherwise.

4. Numerical results

We now show how measuring the winding angle and the pair-connectedness on the domains of the coarsening IM highlights that the morphological properties of the domain patchwork are those of critical percolation.

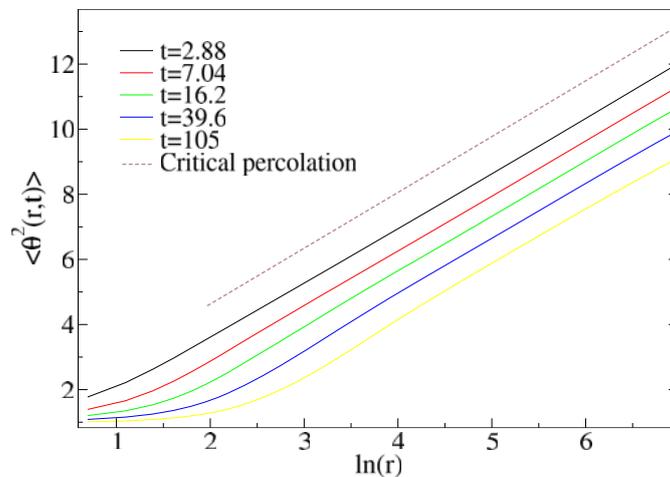


Figure 1. Average squared winding angle for the domains of the largest cluster of the pure $2d$ IM, plotted against $\ln r$, the distance r along the hull. Results are relative to a lattice with $L = 640$. In the key we report the measurement times. The dashed line is Eq. (5) with $k = 6$, the value of critical percolation.

In Fig. 1 we report results for the clean model of size $L = 640$, for various measurement times. The dashed blue line is the analytical curve, namely Eq. (5) with $k = 6$.

Apart from an upward vertical shift of the curves for increasing measurement times – whose interpretation is discussed in [8] – for each curve we observe two behaviors: an initial part (short distances) in which the analytical expression is not followed, and a large-distance regime where numerical data are very well described by Eq. (5). Indeed, we fitted the slope of the purple curve corresponding to $R(t) = 2.68$ and $t = 3.13$ in the range $4 < \ln(x) < 7$, and we obtained $k = 5.94$, in excellent agreement with the value $k = 6$ for critical percolation. This

signals that over sufficiently large distances the largest cluster has the morphological properties of percolation. Interestingly, we see that the crossover between the two behaviors takes place at a distance l_t which increases with the measurement time.

We find a similar behaviour for pair-connectedness, shown for the pure IM in Fig 2. We performed the measurement of $g(r)$ at different times on a system of size $L = 512$. For each curve except $t = 2$, after an initial distance which increases with time, curves for coarsening have the same slope as that for percolation, the black line with slope $-2\Delta = -10/48$ (at large distances the curves bends upward as due to finite size effects). Notice that this is not true for very small times, when the system is still very close to the initial condition. The vertical shift of the curves for varying measurement times is interpreted in [8] in the same way as for the winding angle.

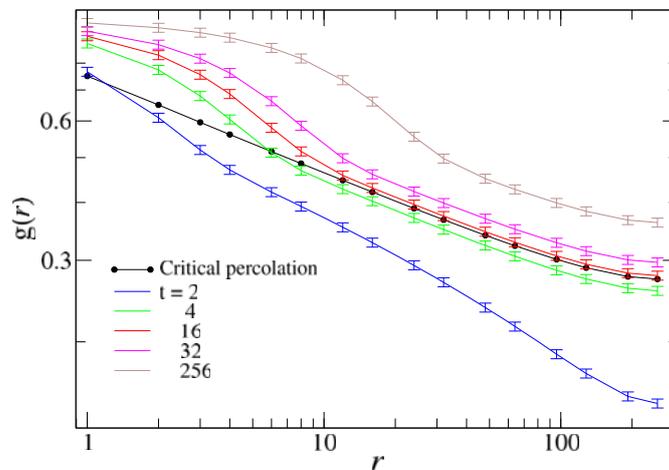


Figure 2. Pair connectivity measured on a lattice at percolation threshold (black line) and for a coarsening homogeneous $2d$ IM (colored lines) is plotted against the distance r . Measurement times are given in the key. The lattice size is $L = 512$ in both cases.

In Figs. 1 and 2 we noticed a length, growing with time, after which the domains acquire the morphological properties of critical percolation. It is natural to identify this length with the growing length $R(t)$, the typical size of the correlated regions (domains). Indeed, as mentioned in Sec. 1, percolative properties can only be present a length scale over which the system is still uncorrelated. This interpretation can be formalised and quantitatively verified through scaling arguments [8].

Most importantly, we find analogous results for all the values of disorder strength considered, for both RFIM and RBIM. We only report data for the RFIM with $\epsilon = 1$ in Figs. 3 and 4

We regard this as compelling evidence that the clusters arising in the coarsening process *are* those of critical percolation, for both pure and disordered systems. We can therefore conclude that percolation effects are quite robust, since they are not destroyed by the presence of the considered quenched disorder.

5. Conclusions

In this work we have investigated the relevance of percolative effects on the coarsening process of the $2d$ IM quenched from a completely disordered initial state to zero final temperature. We focused on the clean case and on two forms of quenched randomness, random bonds and random fields. We have used two quantities – winding angle and pair-connectedness – which represent efficient tools to detect percolation effects.

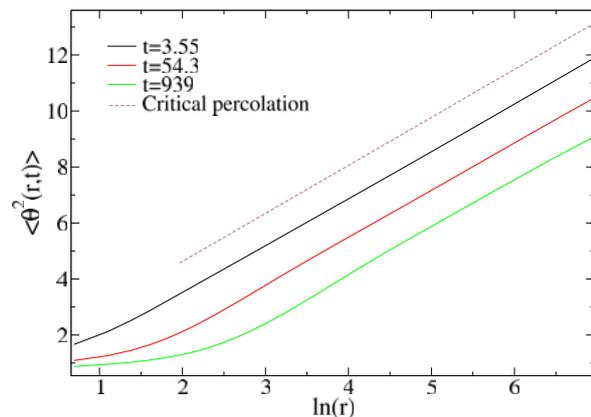


Figure 3. Same as Fig. 1, but for RFIM with $\epsilon_{RF} = 1$.

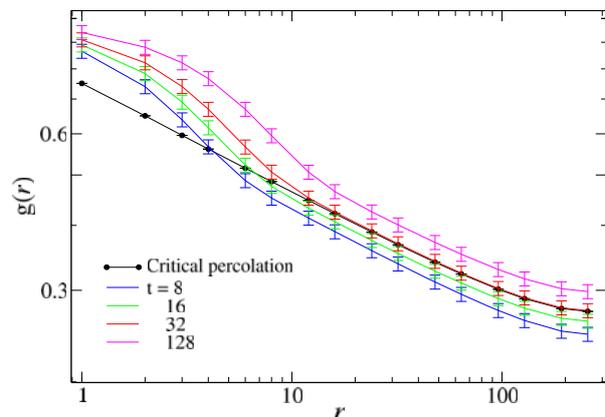


Figure 4. Same as Fig. 2 but for a RFIM with $\epsilon_{RF} = 1$.

In the light of our results, we can conclude that the influence of percolation on the coarsening dynamics of a quenched ferromagnet – previously highlighted for homogeneous models – also extends to systems where quenched disorder is present, systems that are much less understood. These results represent a first necessary step toward the generalisation of one of the few analytical theories of coarsening [18] – currently available for pure systems – that hinges on the percolative properties of the domains of the ordering system.

Finally, a natural extension of this work concerns randomly diluted models, a class of systems whose phase ordering kinetics presents subtleties and differences with respect to random field and random bond models [19].

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