On the onset of the percolating cluster in the Ising model after a temperature quench

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After a sudden quench from the disordered high-temperature \( T_0 \to \infty \) phase to a final temperature below the critical point \( T_F < T_c \), the non-conserved kinetics of the two-dimensional ferromagnetic Ising model (2dIM) initially approaches the critical percolation state before entering the coarsening regime. This approach involves two timescales associated with the first appearance (at time \( t_{p_1} \)) and stabilization (at time \( t_p \)) of a giant percolation cluster, as previously reported, but nonetheless, the microscopic mechanisms that control such timescales are not yet fully understood. In this paper we study the role of the different microscopic mechanisms on each time regime after the quench \( (T_F = 0) \) by distinguishing between spin updates that decrease the total energy of the system from those that keep it constant, the latter being parametrized by the probability \( p \). We show that the cluster size heterogeneity \( H(t, p) \) and the typical domain size \( \ell(t, p) \) have no dependence on \( p \) in the first regime up to \( t_{p_1} \), thus indicating that the emergence of the first percolating cluster is completely driven by energy decreasing updates. On the other hand, the time for stabilizing a percolating cluster is controlled by the acceptance rate of constant-energy updates: \( t_p(p) \sim p^{-1} \) for \( p \ll 1 \) (at \( p = 0 \), the dynamics gets stuck in a metastable state). These updates are also the relevant ones in the later coarsening regime where dynamical scaling takes place. Because the phenomenology on the approach to percolation point is universally shared by 2d systems with a non-conserved kinetics and certain cases of conserved kinetics as well, our results may suggest a simple and effective way to set, through the dynamics itself, \( t_{p_1} \) and \( t_p \) in such classes of systems.

I. INTRODUCTION

After being equilibrated at a high temperature \( (T_0 \to \infty) \) and suddenly quenched to a temperature well below the critical one, \( T_F \ll T_c \), the non-conserved order parameter dynamics of the ferromagnetic 2d Ising model first approaches the percolation critical point \( [1, 4] \), to then follow a curvature-driven, coarsening dynamics in which the spatial structure is statistically invariant once distances are measured with the lengthscale \( \ell(t) \) associated with the clusters linear size, i.e., dynamical scaling \( [5] \). These two temporal regimes are connected, what has led to several predictions that were experimentally verified in liquid crystals \( [6, 7] \) (see the latter reference for a recent and more detailed report on the universal features of the curvature-driven dynamics in these experiments). Moreover, sharing the geometrical properties of the critical percolation state has a fundamental influence on the late stages of the dynamics, where the asymptotic state may be fully magnetized or divided into parallel stripes \( [8, 13] \). The late-time growth of order during the coarsening regime is clearly different from that ruling the development of the stable, giant cluster that characterizes the critical percolation threshold. The first spanning cluster, formed at \( t_{p_1} \), is not stable against the fluctuations still present in the system, despite the absence of activated processes. It will break and regrow multiple times while competing with the second largest cluster, until at least one of them stabilizes at the timescale \( t_p \sim L^{z_p \approx 3} \) \( [3, 4] \) when the system approaches the percolation critical point. The exponent \( z_p \) encodes the lattice-geometry dependence and, for the square lattice, it has been argued that \( z_p = 2/5 \) \( [4] \). It is only after this time that the asymptotic power-law behavior associated with the curvature-driven growth starts \( [4] \). The main objective of this paper is to study the role of different microscopic mechanisms associated with these two timescales and the formation of the first percolating cluster and its subsequent stabilization.

The geometric description of the 2d ferromagnetic Ising model equilibrium states is relatively simpler at temperatures well below and well above \( T_c \). In these temperature regimes, connected groups of parallel spins (clusters or domains) have a small size diversity. At temperatures \( T \ll T_c \), the system is dominated by a single large, percolating cluster. Due to the weak thermal fluctuations, there is also a few small clusters, whose size distribution decays exponentially. In the other temperature limit, \( T \gg T_c \), large domains are destabilized by

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the thermal noise and the system is populated by small clusters whose size distribution is, once again, a decreasing exponential. It is only close to $T_c$ that the diversity of sizes increases and the size distribution broadens, approaching a power-law. In the thermodynamic limit, $L \to \infty$, the domain size distribution for a single sample becomes dense at all temperatures, i.e., the position of the first missing cluster size also diverges. In contrast, for a finite sample, the distribution is dense only below a certain cluster size, sparse after it. The non homogeneity of the clusters may be quantified by the so-called cluster size heterogeneity $H$, the average number of distinct cluster sizes occurring in a finite sample, irrespective of the number of domains that are equally large. This observable was studied in percolation \[14\,16\], spin equilibrium models \[17\,19\] and recently extended to out-of-equilibrium \[20\] and more general contexts \[21\]. The rich behavior of the time-dependent heterogeneity, $H(L,t)$, confirms that it may be useful to understand the interplay between percolation and coarsening dynamics. For simplicity, from now on we will omit the size dependence and write $H(t)$ (analogously for the equilibrium counterpart).

Quenching the system from $T_0 \to \infty$, the dynamical heterogeneity $H(t)$ presents a very pronounced peak at the beginning of the dynamics \[20\]. After the quench, correlations start building larger clusters, the domain-size distribution widens and the growth of $H(t)$ is a consequence of the larger size diversity. At the same time, the first spanning cluster starts building up, taking most of system size. Because less space remains for the other clusters, their number and size decrease, and along with them, the system diversity. These two competing mechanisms explain the peak of $H(t)$ occurring slightly before $t_{p_1}$, the time when the largest cluster percolates \[3\,4\]. Despite the longer timescales, an analogous precursor behavior was also observed for the Voter model \[20\], whose dynamics, without surface tension, is much slower \[22\,23\]. The dynamical heterogeneity $H(t)$ presents three well separated regimes: a peak immediately after the quench in temperature, followed by an incipient plateau and, eventually, the power-law decaying. These correspond, respectively, to the appearance of the first percolating cluster, the stabilization of the largest cluster (and the approach to the percolation critical point) and, finally, the coarsening, curvature-driven growth \[20\]. The approximated analytical results of Ref. \[20\] well explained the height of the plateau and the exponent of the later regime. They are, however, valid only after the dynamics has approached the percolation critical point and do not explain the peak of $H(t)$ and the region around it. Particularly interesting is the universality of its height: not only it is the same for both the Ising and the Voter model after the quench but also very close to the maximum found in Ref. \[19\] for the equilibrium heterogeneity at a temperature well inside the paramagnetic phase (there is a second, smaller peak very close to $T_c$). As will be discussed in the next sections, other instances of this universality appear related with the nature of different spin flips.

We are interested in the role played by the microscopic mechanisms in building and stabilizing the percolating structures in the early time regime. If we take the temperature quench to $T_F = 0$, only spin updates that either decrease ($\Delta E < 0$) or keep the energy constant ($\Delta E = 0$) are allowed. In particular, how does the characteristic time to attain the percolation critical point depends on these processes? Since in the curvature-driven regime domain coalescence does not occur, how does the percolating cluster first appear? In the next section we describe the model and the methods in more detail while in Sec. \[III\] we present new results for the size heterogeneity $H(t)$ and the average linear size $\ell(t)$ of the geometric clusters (connected regions of aligned spins). Finally, in Sec. \[IV\] we summarize and discuss our results.

II. MODEL AND METHODS

Starting from an initial state with uncorrelated spins (infinite temperature) having an equal probability of being $\pm 1$, we study the ferromagnetic 2d Ising model after a quench to $T_F = 0$. The Hamiltonian is

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j,$$

(1)

where $J > 0$, $\sigma_i$ is the spin at site $i$ and the sum is over all nearest neighbors pairs on an $N = L \times L$ square lattice with periodic boundary conditions. The simulations were performed with linear sizes up to $L = 5120$. After the quench, the system evolves through a continuous time, single-spin dynamics \[24\].

In the zero-temperature dynamics, a site is randomly selected and the local field (the sum of the spins of the neighboring sites) is computed. If, by flipping, this spin becomes aligned with the local field, the energy change is $\Delta E < 0$ and the movement is accepted with probability 1. If $\Delta E > 0$, i.e., the spin becomes anti-aligned with the local field, the movement is rejected and the spin is left unchanged. When the flip does not change the energy of the system, $\Delta E = 0$, it is accepted with probability $p$ in order to assess the role of each type of update. For the heat bath and Glauber dynamics, $p = 1/2$, while for the Metropolis algorithm, $p = 1$ \[24\]. In the constrained case $p = 0$, only energy-lowering movements are accepted \[25\,26\]. In the continuous-time dynamics \[24\], we keep a list of the $N_{mobile}$ spins that may flip, i.e., those with $\Delta E \leq 0$ and, after each attempt of flipping one spin from this list, the simulation time is incremented by $1/N_{mobile}$ and the list is updated. In the continuous-time dynamics \[24\], we keep a list of the $N_{mobile}$ spins that may flip, i.e., those with $\Delta E \leq 0$ and, after each attempt of flipping one spin from this list, the simulation time, measured in Monte Carlo steps (MCS), is incremented by $1/N_{mobile}$ and the list is updated. Time is measured in Monte Carlo steps...
(MCS), where one unit corresponds to $N_{\text{mobile}}$ attempts to flip. Averages up to 10000 samples were taken for the smaller systems, while larger sizes require fewer samples (1000).

### III. RESULTS

![Graph](image)

**FIG. 1:** Dynamical cluster heterogeneity $H(t)$ versus time (in MCS) after a quench from $T_0 \to \infty$ down to $T_F = 0$, for several values of $p$ (the flipping probability when $\Delta E = 0$). The system linear size is $L = 1280$. The time a percolating cluster first appears is indicated by $t_{p_1}(p)$ (dark squares) and there is almost no dependence on $p$. The time that the percolating cluster stabilizes, $t_p(p)$ (dark circles), on the other hand, decreases with $p$. In the first regime, $t \lesssim t_{p_1}$, all curves collapse and $H(t)$ is independent of $p$, differently from the interval $t > t_{p_1}$, where there is a strong dependence on it. Notice that the height of the peak of $H(t)$ coincides with the high temperature peak ($T_2 > T_1$) observed for the equilibrium measure of $H$, indicated by a horizontal line. The inset shows $t_p(p)/t_p(1)$, that seems to have a power-law dependence on $p$ as $p$ decreases, $1 + p^{-1}$ (solid line). However, above $p \sim 0.5$, $t_p(p)$ barely depends on $p$ and $t_p(p) \simeq t_p(1)$.

The initial, equilibrium state at $T_0 \to \infty$ has uncorrelated spins forming small domains that are similar in size. The corresponding heterogeneity is $H(t = 0) = H_{\text{eq}}(\infty)$, where $H_{\text{eq}}(T)$ is the equilibrium heterogeneity at the temperature $T$. This initial state has a large number of spins with at least half of their neighbors oriented in the opposite direction, i.e., such that putative flips have $\Delta E \leq 0$. These spins are associated with rough surfaces that may become smoother and with small clusters that may disappear (with less holes, the embedding clusters get more compact) or coalesce after a quench. With the growth of the domains, their size distribution becomes wider and, consequently, $H(t)$ increases. Soon after the quench from $T \to \infty$ to zero temperature, there is a peak in $H(t)$ [20] as shown in Fig. 1. The peak occurs within the first MCS, just before a percolating cluster appears for the first time at $t = t_{p_1}$. As observed in Ref. [20], the height of the peak has some degree of universality and is very close to the dynamical peak for the Voter model and for the largest peak of the equilibrium measure $H_{\text{eq}}(T)$ for the Ising model that occurs well above $T_c$. The latter is indicated, in Fig. 1 by a small horizontal line. In Ref. [21] it was argued that an upper bound for $H$ is obtained when $N$ is divided into smaller domains in a deterministic way: one cluster of each size, starting from 1, until the system is fully covered. Obviously, for stochastic systems this bound is never approached either because of repeated sizes or too large clusters that decrease their total number. The fact that the heterogeneity, in the several situations described above, reaches a similar maximum is related to getting as close as possible of this upper limit in the presence of stochasticity. Also remarkable is that not only the height of the peak, but the whole region up to $t_{p_1}(p)$ does not depend on $p$, i.e., on the dynamics. Since $p$ is associated with the $\Delta E = 0$ updates, this is an indication that the energy-conserving flips, although present, do not seem to play an important role in the early dynamics.

![Graph](image)

**FIG. 2:** Growing length scale $\ell(t)$, as a function of time (in MCS), after a temperature quench from $T_0 \to \infty$ down to $T_F = 0$ for several values of $p$ and $L = 1280$. Dark squares and circles locate, respectively, $t_{p_1}(p)$ and $t_p(p)$. The straight solid line indicates the power-law $t^{1/2}$, characteristic of the coarsening regime. The initial exponential growth of $\ell(t)$, indicated by a thin solid line, extends up to the peak of $H(t)$. Inset: local slope, $\alpha = d \log \ell(t)/d \log t$, as a function of time (semi-log scale).

For the random initial condition that we consider, the behavior of $H(t)$ strongly depends on $p$ between $t_{p_1}(p)$ and $t_p(p)$, the regime in which the percolating cluster stabilizes, and beyond, Fig. 1. For $p = 0$ the dynamics is halted, never entering the coarsening regime [13, 28], and $H(t)$ attains a plateau. This blocking of the dynamics also occurs in lattices with an odd coordination, as the honeycomb [29]. Deviations from this plateau are already seen even for very small values of $p$ and the larger $p$ is, the earlier the departure from the plateau occurs. Therefore, energy-lowering flips alone are not enough to stabilize the percolating cluster and, eventually, to enter the curvature-driven growth regime. As $p$ goes from 0 to 1, increasing the acceptance rate of energy conserving flips, the time interval between $t_p(p)$ and $t_{p_1}(p)$ decreases,
i.e., the percolating cluster stabilizes faster. The minimum $t_p$ occurs for $p = 1$ and the inset on Fig. 3 shows that although there is little or no dependence for $p > 0.5$, below this value it increases very fast, $t_p(p) \sim p^{-1}$.

![FIG. 3: Relation between the $H(t)$ and the growing length $\ell(t)$. Notice that even the $p = 0$ case is collapsed onto the universal curve (in this case, however, the curve is interrupted at the maximum value of $\ell(t)$). The scaling is very good, with small deviations occurring close to $t_{p1}$, as can be seen in the inset.](image)

It is also interesting to compare the behavior of $H(t)$ with the growth of a lengthscale associated with the average radius of the domains after the quench, $\ell(t)$. The main panel of Fig. 2 shows this growing length for several values of $p$ while the inset presents the corresponding instantaneous declivity, i.e., the exponent $\alpha(t) = \log \ell(t)/\log t$. Initially, the growth is exponential (indicated by a thin solid line) and, like the heterogeneity $H(t)$, $\ell(t)$ has no dependence on $p$ up to $t \simeq t_{p1}$ and all curves are collapsed. For $p = 0$, $\ell(t)$ attains a constant value, whereas the case $p = 1$ has the fastest growth. If $p \neq 0$ and for times larger than $t_p(p)$, the dynamics approach the coarsening regime where $\ell(t) \sim t^{1/2}$. The main panel of Fig. 2 shows that, in this late regime, $\ell(t)$ is parallel to the thick solid line while, in the inset, it corresponds to the plateau at $\alpha \simeq 1/2$. Notice that the coefficient decreases with $p$ and the curves, albeit parallel, are displaced. It is in the intermediate regime, roughly between $t_{p1}(p)$ and $t_p(p)$, that the dependence on $p$ has a larger impact. This is an indication of how important the energy-conserving updates are for the stabilization of the percolating cluster. For $p \geq 0.5$, the dynamics accelerates after $t_{p1}$ up to a maximum (e.g., for $p = 1$, $\alpha \sim 0.6$ at its largest value), and then decreases approaching 0.5. Further decreasing $p$, the maximum moves toward $t_{p1}$ and a minimum develops and becomes deeper, eventually attaining $\alpha = 0$ as $p \to 0$.

When, instead of the time, we use the characteristic length $\ell(t)$ as the independent variable, Fig. 3 a very good collapse is obtained for the curves with different values of $p$. Notice that even $p = 0$ is included, but in this case the curve is interrupted when the plateau is attained. Some deviations from the scaling are observed around $t_{p1}$, the beginning of the intermediate region (inset). Before $t_{p1}$, the collapse is a direct consequence of both $H(t)$ and $\ell(t)$ being independent of $p$, as shown in Fig. 1. This is not, however, the case at larger times where there is a strong $p$-dependence and all curves are different. The overall shape of $H(t)$ and the diverse regimes have been discussed in Ref. [20], including the power-law tail associated with the coarsening regime.

![FIG. 4: Density of spins whose flip would decrease the energy, $n_<(t)$, or keep it constant, $n_=(t)$, as a function of time, for $p = 0$ (purple symbols) and $p = 1$ (orange symbols). The system linear size is $L = 1280$. Indeed, coarsening does not occur for $p = 0$: $n_<(t)$ vanishes exponentially and the dynamics is blocked soon after $t_{p1}$. For $p > 0$, $n_<(t) \sim t^{-1/2}$ and $n_=(t) \sim t^{-3/2}$ for $t \gg 1$.](image)
of clusters linearly decreases with time while \( R \) increases as \( t^{1/2} \), one may estimate \( n_{<}(t) \sim RN_{c} \sim t^{-1/2} \). On the other hand, the main contributions to \( n_{<} \) come from large clusters, i.e., those whose areas are much larger than the typical ones (\( A \gg \lambda t \), with \( \lambda \simeq 2 \)). Once the area is much larger than the instantaneous correlation length, many spins in the domain are uncorrelated. Because of that, these large domains preserve some memory of the random initial state, being less compact and with a rough interface. We estimate \( n_{<}(t) \) considering the contributions from dangling ends,

\[
n_{<}(t) = \int_{A_{0}}^{L^{2}} f(A, t)n(A, t)\, dA,
\]

where \( A_{0} \) is a microscopic area and \( n(A, t)\, dA \) is \([2]\) the average density of clusters with area between \( A \) and \( A + dA \) already in the coarsening regime (\( t \gg t_{p} \)),

\[
n(A, t) \simeq \frac{2c_{d}(\lambda t)^{\tau-2}}{(A + \lambda t)^{\tau}}, \quad A_{0} \ll A \ll L^{2},
\]

de \( c_{d} \) is a small constant and \( \tau = 187/91 \). The fraction \( f(A, t) \) is the ratio between the average number of spins with \( \Delta E < 0 \) in a cluster of area \( A \) at the time \( t \) after the quench (\( N_{c} \)) and the number of spins in the cluster (\( A/A_{0} \)), \( f(A, t) \sim N_{c} A_{0}/A \). The more irregular the perimeter is, the larger is \( N_{c} \). From the area-perimeter relation \( A \sim p^{\alpha} \) (\( \alpha = 2 \) for regular domains while irregular ones have \( \alpha < 2 \)), we assume that \( N_{c} \) is given by deviations from the regularity, i.e., \( N_{c} \sim (p/\ell_{0})^{2-\alpha} \), where \( \ell_{0} \) is a microscopic length. Thus

\[
f(A, t) \sim \left( \frac{p}{\ell_{0}} \right)^{2-\alpha} \frac{A_{0}}{A} \sim A^{1/\alpha}(\lambda t)^{1/2-\alpha},
\]

where the area-perimeter relation was extended \([2]\) to include time,

\[
\frac{A}{\lambda t} \sim \left( \frac{p}{\lambda t} \right)^{\alpha}.
\]

For large clusters (\( A \gg \lambda t \)), those that indeed contribute most for \( N_{c} \), \( \alpha \simeq 1 \). Using this value, and substituting Eq. (4) into Eq. (2), we obtain \( n_{<}(t) \sim t^{-3/2} \). Nonetheless, we notice, Fig. 4 that when the power-law regime settles (\( t > t_{p} \)), \( n_{<}(t) \ll n_{=} \), the flips that decrease the energy are much less frequent, and thus less relevant in this regime, than those that keep it constant.

We also studied the different asymptotic states, either the ground state or a set of parallel stripes, and how the corresponding probabilities depend on \( p \) (except, of course, for \( p = 0 \)). Within the error bars, our results (not shown) are essentially constant and compatible with those for \( p = 0.5 \) \([10, 11]\) and 1 \([12]\).

**IV. CONCLUSIONS**

When the ferromagnetic 2d Ising model is taken out of equilibrium by a sudden decrease in temperature, from \( T_{0} \rightarrow \infty \) to \( T_{F} \rightarrow 0 \), the first lengthscale that appears is related to the percolation critical point to which the system is attracted on a timescale \( t_{p} \). At a longer timescale, the system enters the coarsening regime in which the dynamics is driven by the curvature of the domains and dynamical scaling is known to hold. We here studied this scenario through the cluster size heterogeneity \( H(t) \) and the average cluster linear size \( \ell(t) \), trying to uncover the role played by the spin flips that either decrease or keep the energy constant under the non conserved order parameter dynamics. Those updates that reduce the energy are always accepted while those that do not change it, the entropic flips, have a probability \( p \).

The short-time dynamics, up to the time \( t_{p} \), when the first percolating cluster appears, is independent of \( p \). Indeed, the results are all equivalent, even when completely suppressing the constant-energy flips (\( p = 0 \)). In this initial regime, spin flips with \( \Delta E = 0 \) play no relevant role on the construction of the first percolating cluster, differently from the coalescence processes driven by the energy-lowering spin flips. It is indeed the coalescence of small domains that explain the exponential growth that leads to the first cluster spanning the whole system. This initial percolating cluster only becomes stable at a much larger time (\( t_{p} \)), when the system approaches the percolation critical point. The larger the probability of accepting energy conserving flips is, the sooner this point is attained and the system enters the coarsening regime. Instead, when these flips are suppressed, \( p \ll 1 \), \( t_{p}(p) \sim p^{-1} \). The fact that the timescale associated with the stabilization of the percolating cluster is the inverse of the probability of the constant energy flips occurring is the confirmation that these flips are the solely responsible for this process, the energy decreasing flips being important only for its initial formation. Notice also that these flips dominate the curvature-driven regime, and the system only enters the dynamical scaling after \( t_{p} \). We argued that, in the scaling regime, \( n_{<}(t) \sim t^{-3/2} \) while \( n_{=} \sim t^{-1/2} \), exponents whose values are completely consistent with those obtained in the simulations. From Refs. \([3, 4]\), \( t_{p} \) depends on the system size as \( t_{p} \sim L^{z_{p}}, \) where it was conjectured that \( z_{p} = 2/5 \) for the square lattice. It is still an open question whether \( z_{p} \) depends on \( p \). Combining with our result, we may write \( t_{p}(L, p) \sim L^{z_{p}}/p \), As we lower \( p \), the dynamics gets slower because fewer proposed zero-energy flips are accepted. When \( p = 0 \), the system freezes soon after \( t_{p,1} \), meaning that there are no \( \Delta E < 0 \) flips available and the configuration is blocked.

The importance of the early approach to critical percolation to the ensuing dynamics and the geometric properties of clusters and interfaces have been emphasized and recognized in the last years. Although we only considered here the non-conserved order parameter dynamics (Model A), the approach to the percolation point also occurs for symmetric mixtures (50:50) the model B dynamics that conserves the order parameter \([30, 32]\). Understanding how \( t_{p} \) depends on \( p \) in this case may be relevant for a multitude of phase separating systems. Moreover,
it is possible to devise protocols that change the value of \( p \) along the dynamics. For example, the system may first evolve with a constrained dynamics (\( p = 0 \)), commonly observed in glassy systems and colloidal suspensions \(^{33}\), until a metastable state is attained. From that state on, it may evolve following the chosen \( p(t) \) protocol in order to study, for example, the yield to scape from metastable states and the role of memory in the reorganization of the geometrical structures. Whatever the dynamics is, it would be interesting to find ways to mimic the effect of \( p \) on experimental setups. In addition, it would be important to access the universality of those results on lattices with different coordination numbers such as the triangular one and on different systems such as the Potts \(^{34,35}\) and Voter models \(^{20,22,23,36}\).

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