Freezing into Stripe States in Two-Dimensional Ferromagnets and Crossing Probabilities in Critical Percolation

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When a two-dimensional Ising ferromagnet is quenched from above the critical temperature to zero temperature, the system eventually converges to either a ground state (all spins aligned) or an infinitely long-lived metastable stripe state. By applying results from percolation theory, we analytically determine the probability to reach the stripe state as a function of the aspect ratio and the form of the boundary conditions. These predictions agree with simulation results. Our approach generally applies to coarsening dynamics of non-conserved scalar fields in two dimensions.

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We investigate the fate of a kinetic two-dimensional Ising ferromagnet following a quench from above the critical temperature to zero temperature. Intriguingly, this evolving system can sometimes get trapped in an infinitely long-lived metastable stripe state that spans the system vertically or horizontally [1, 2, 3]. The case of two dimensions is special; in one dimension the system always reaches the ground state, while in three or more dimensions the ground state is never reached [1].

In this Letter we propose exact probabilities for a two-dimensional Ising system to reach this metastable stripe state. Our argument should apply to any curvature-driven coarsening process with a non-conserved scalar order parameter, such as the time-dependent Ginzburg-Landau equation [4, 5, 6]. For a square system, the probability to get trapped in a vertical or a horizontal stripe state was previously estimated [1, 2] to be close to 1/4. Here we exploit the relation between coarsening and critical percolation to argue that this probability equals 1/8 = 2/27 ln 27/16 = 0.3558... for a system with free boundary conditions; the corresponding freezing probability for periodic boundary conditions is found to be 0.3390... .

Our approach is based on two key ingredients:

(i) Soon after the quench, the characteristic domain length scale ℓ becomes substantially larger than the lattice spacing a while remaining much less than the system size: L, a ≪ ℓ ≪ L. At this stage, the domain mosaic has reached the critical point of continuum percolation (Fig. 1(a)), as previously observed in various two-dimensional systems [7, 8].

(ii) During the coarsening regime, ℓ(t) ≫ a, the dynamics becomes deterministic and domain wall evolution is driven only by local curvature [4, 5, 6]. Thus the global domain topology does not change once the coarsening regime is reached [9].

These features imply that the ultimate fate of the system is pre-determined once the critical percolation state is reached. For instance, if a domain exists that crosses the system only horizontally or only vertically, a stripe state is reached. Figure 1 shows an example of a vertical spanning domain shortly after the quench that ultimately coarsens into a vertical stripe; conversely, a domain mosaic that spans in both horizontally and vertically coarsens into a ground state.

While individually the observations (i) and (ii) are known, their combined use leads to analytical predictions for the fate of two-dimensional Ising ferromagnets. The connection with the critical state of continuum percolation is central as it allows us to use exact results about crossing probabilities to determine the final state of the Ising system. These quantities are defined as the probabilities for the existence of a spanning cluster with a specified topology. We denote these crossing probabilities for free and periodic boundary conditions as F and P, respectively. For a critical rectangular system with aspect ratio r (ratio of height to width) [10], the crossing probabilities are non-trivial (i.e., strictly between 0 and 1), universal functions of r [11, 12]. Beautiful exact expressions for various crossing probabilities were originally calculated via conformal field theory [13, 14, 15, 16], and some of them have been proved in Refs. [17, 18, 19].

The connection (i) with critical percolation may seem surprising since the initial state (with equal numbers of up and down spins) is not critical; on the square lattice, the up spins percolate when their density exceeds p_c ≈ 0.3927. Hence initially neither phase percolates. However the system quickly approaches the critical state of continuum percolation in which the crossing probabilities are non-trivial. To appreciate this property, consider for concreteness domain coarsening in the square geometry with free boundary conditions. Let F_v be the probability that a spin up domain crosses vertically (with no constraint on horizontal crossing); F_v also equals the horizontal crossing probability (because the system is square), and further equals the crossing of spin down domains (due to up/down symmetry). A vertical spanning spin up domain exists if and only if a horizontal spanning spin down domain does not. (This last statement is predicated on the non existence of singular points in which more than two domains meet, see Fig. 2.) Hence F_v = 1 − F_v, so that F_v = 1/2, which is indeed non-trivial.

We begin with the analytically simpler case of free
Moreover, the exact form of $F$ spin up (gray) or spin down (black). A spanning spin-up domain, that eventually coarsens into a vertical stripe, is highlighted.

FIG. 2: (a) A state where 4 Ising domains meet at a single point evolves into a state (b) where only two domains can meet under zero-temperature single-spin flip dynamics.

boundary conditions. In this setting, every domain mosaic either spans only vertically, only horizontally, both horizontally and vertically (dual spanning), or the mosaic does not contain a spanning cluster. Their respective probabilities, $F_{hv}$, $F_{h\pi}$, $F_{hv}$, and $F_{hv}$ (the dual-spanning and non-probabilities are identical by up/down symmetry) therefore satisfy the normalization condition

$$F_{hv} + F_{h\pi} + 2F_{hv} = 1.$$  \hspace{1cm} (1)

Moreover, the exact form of $F_{hv}$ is known to be \[15, 16\]

$$F_{hv}(r) = \frac{\sqrt{3}}{2\pi} \lambda 3 F_2 \left(1, 1, \frac{4}{3}, \frac{5}{3}; 2; \lambda \right),$$ \hspace{1cm} (2)

where $p F_q(a_1, \ldots a_q; b_1, \ldots b_q; \lambda)$ is the generalized hypergeometric function \[20\], $\lambda = \lambda(r)$ is defined implicitly by

$$\lambda = \left(1 - k \right)^2, \hspace{1cm} \text{with} \hspace{1cm} r = \frac{2K(k^2)}{K(1 - k^2)},$$

and $K(u)$ is the complete elliptic integral of the first kind \[20\].

The corresponding horizontal crossing probability follows by symmetry

$$F_{h\pi}(1/r) = F_{hv}(r).$$ \hspace{1cm} (3)

while the crossing probability for dual spanning satisfies

$$F_{hv}(r) = \frac{1}{2} (1 - F_{hv}(r) - F_{h\pi}(r)) = F_{hv}(1/r).$$ \hspace{1cm} (4)

The basic relation between Ising domains and critical percolation implies that, e.g., the crossing probability $F_{hv}$ coincides with the probability for the Ising system to freeze into a vertical stripe state as a function of $r$.

To test this basic prediction for the freezing probability, we simulate the kinetic Ising model at zero temperature using single-spin flip dynamics with the Metropolis acceptance criterion — a spin is flipped if its energy decreases or remains the same as a result of the flip. To make this simulation more efficient, a list of “active” spins — those whose energy will not increase upon being flipped — is maintained and constantly updated during the dynamics. In each update step an active spin is chosen at random and flipped. One Monte Carlo step corresponds to each active spin flipping once, on average.

We simulate many quenches from $T = \infty$ to 0 on lattices of dimension $(256/r) \times 256$. For each value of $r$, we performed $2 \times 10^4$ simulation runs, with each starting from a different random initial condition. We define a domain as a connected cluster of nearest-neighbor aligned spins. Clusters are identified using a cluster multilabeling method \[21\]. To determine whether a quenched system ultimately freezes into a stripe state, one should, in principle, simulate until the system ceases to evolve. The final stages of the evolution take a disproportionately large amount of CPU time, however, and it is advantageous to stop the simulation when the domain mosaic first reaches its final state topology. For this Ising system, our simulations indicate that after 200 Monte Carlo steps, domain mosaics have reached the topology of the final state with a probability that exceeds 0.998. Thus we may identify the state of the system at this early time as the predictor of the topology in the final state.

Figure 3 shows our numerical results for the probability for a specified ultimate fate of an Ising system with free boundary conditions for a variety of aspect ratios
FIG. 3: Probabilities of various domain topologies in the kinetic Ising model following a quench with free boundary conditions: vertical stripes (+), dual-spanning configurations (□), and horizontal stripes (×). Error bars are about 1/3 the symbol size. The lattice dimensions are $(256/r) \times 256$ for various aspect ratios between 0 and 1. Also shown are the corresponding exact percolation crossing probabilities $P_{\nu\nu}$, $P_{hv}$, and $2P_{hv}$, respectively, from Eqs. (3) and (4).

FIG. 4: Probabilities of various domain topologies in the kinetic Ising model following a quench with periodic boundary conditions: vertical stripes (+), dual-spanning configurations (□), and horizontal stripes (×), with error bars about 1/3 of the symbol size. The lattice dimensions are $(256/r) \times 256$ for aspect ratios between 0 and 1. Also shown are the corresponding exact percolation crossing probabilities $P_{1,0}$, $P_{0,1}$, and $2P_X$, respectively, from Eqs. (6) and (7).

These agree well with the exact crossing probabilities that follow from Eqs. (2)–(4). For the important special case of a square geometry, $r = 1$, Eq. (2) can be simplified to

$$P_{h\nu}(1) = P_{\nu\nu}(1) = \frac{1}{4} - \frac{\sqrt{3}}{4\pi} \ln \frac{27}{16} = 0.1779 \ldots$$

from which the probability of the Ising system coarsening into a stripe state equals $2P_{h\nu}(1) = 0.3558 \ldots$. An earlier numerical estimate for the probability of reaching a stripe state $[14]$ is consistent with this exact result.

For periodic boundary conditions, a parallel set of results can be constructed to again connect the ultimate fate of the Ising system and percolation crossing probabilities. The nature of the crossing probabilities is substantially more complex for systems with periodic boundaries because spanning clusters can wrap around the torus multiple times in the vertical and horizontal directions. There are two types of spanning clusters $[14, 23, 24]$. “Winding” clusters are labeled by their vertical and horizontal winding numbers, $(a, b)$. For example, winding numbers $(0, 1)$ and $(1, 0)$ correspond to a vertical and a horizontal stripe, respectively. A spanning cluster that wraps around the torus once in the vertical direction and once in the horizontal direction can have one of two winding number pairs, $(1, 1)$ or $(1, -1)$, and gives a diagonal stripe configuration when the torus is unwound onto the square. The other cluster type is the “cross topology” in which a spanning cluster is formed by the union of two or more spanning clusters with distinct winding numbers.

Let $P_{a,b}(r)$ denote the crossing probability for a spanning cluster with winding numbers $(a, b)$ to exist on a rectangle with aspect ratio $r$ and periodic boundary conditions. This probability is given by $[14]$,

$$P_{a,b}(r) = \sum_{l \in \mathbb{Z}} \left[ Z_{3al,3bl} - Z_{2al,2bl} - \frac{1}{2} Z_{(3l+1)a,(3l+1)b} - \frac{1}{2} Z_{(3l+2)a,(3l+2)b} + Z_{(2l+1)a,(2l+1)b} \right],$$

(6)

where $Z_{m,n}$ is a shorthand for $Z_{m,n}(\frac{r}{4} ; r)$; generally

$$Z_{m,n}(g ; r) = \frac{\sqrt{g}}{\sqrt{\pi} r^g (e^{\frac{r}{2}})^g} e^{-\pi g (m^2/r + n^2 r)},$$

and $\eta(q) = q^{1/24} \prod_{l \in \mathbb{Z}} (1 - q^l)$ is the Dedekind $\eta$ function $[24]$. Additionally, the configuration with cross topology occurs with probability $[14]$

$$P_X(r) = \frac{1}{2} \left[ Z\left( \frac{8}{3} ; 1 \right) - Z\left( \frac{8}{3} ; \frac{1}{2} \right) r \right],$$

(7)

where $Z(g,f ; r) = \int \sum_{m,n \in \mathbb{Z}} Z_{f m,f n}(g ; r)$. By symmetry, $P_X(r)$ also represents the probability that no cluster spans the system.

To compute the crossing probabilities numerically, it is preferable to employ the asymptotic expansions $[23]$

$$P_{0,1}(r) = 1 - 2\rho^{5/4} + \rho^3 + 2\rho^{12} - 4\rho^{53/4} + 3\rho^{15} \ldots$$

$$P_{1,0}(r) = \sqrt{2r/3} \left( \rho^3 - \rho^{15} - \rho^{27} + 4\rho^{35} \ldots \right)$$

$$P_X(r) = \rho^{5/4} - \rho^3 - 2\rho^{12} + 2\rho^{53/6} - 2\rho^{15} \ldots,$$

where $\rho \equiv e^{-\pi/6r}$, rather than evaluating the special functions directly. These expansions provide an excellent approximation for the entire range of aspect ratio $0 < r < 1$ $[23]$. 

$\eta(q) = q^{1/24} \prod_{l \in \mathbb{Z}} (1 - q^l)$ is the Dedekind $\eta$ function $[24]$.
Again, a domain mosaic characterized by winding numbers \((0,1)\) or \((1,0)\) occurs with probability \(P_{0,1}\) (or \(P_{1,0}\)), as given by Eq. (6), and coarsens into a vertical (or a horizontal) stripe state. Similarly, a mosaic with cross topology occurs with probability \(2P_X\) given by Eq. (7), and coarsens directly into the ground state (either all spins pointing up or all pointing down). However, a domain mosaic can also reach the ground state by the indirect route of first forming a diagonal stripe state with non-zero winding numbers in both directions. As found previously for the specific case of the \((1,1)\) stripe, such states are long lived [1]; namely, they reach the ground state at a time scale that is much larger than the typical coarsening time \(O(L^2)\).

In Fig. 4 we plot the realizations that evolve to a topology with winding number \((0,1)\) or \((1,0)\), or to the cross topology for a variety of aspect ratios \(r\). These again agree well with the exact percolation crossing probabilities that follow from Eqs. (6) and (7). In the specific case of the square system (aspect ratio \(r = 1\)), the probability of reaching an infinitely long-lived stripe state is \(0.3390\ldots\). Because the kinetic Ising model can also evolve to diagonal stripe topologies, \(P_{0,1} + P_{1,0} + 2P_X\) is less than 1.

In conclusion, the probabilities with which Ising ferromagnets freeze into metastable stripe states correspond exactly to crossing probabilities in critical percolation. Our simulation results for the probabilities to reach a specified ultimate fate (Figs. 3 and 4) agree with theoretical predictions. Our approach also applies to arbitrarily-shaped domains and boundary conditions, and also can be used to determine more subtle characteristics, such as the distribution of the number of stripes.

The correspondence with continuum percolation at the critical point depends crucially on the initial state consisting of an equal number of up and down spins. This equality always holds if the system is quenched from equilibrium at an initial temperature that is above the critical point \(T_c\). If, however, the system is in a magnetic field that is switched to zero simultaneously with quenching, or if the initial temperature is below \(T_c\), then the Ising ferromagnet always freezes into the ground state corresponding to the initial majority phase [1]. This behavior immediately follows from the percolation viewpoint. Such a system is above the percolation threshold and there always exists a spanning domain of the majority phase that percolates in both directions. Consequently, the system coarsens into the ground state.

While we focused on the Ising model with zero temperature spin-flip dynamics, our theory applies more generally to phase ordering kinetics in two-dimensional systems with non-conserved scalar order parameter, as well as to quenches to sub-critical temperatures. In the latter case, the coarsening regime requires that \(\xi \ll \ell(t) \ll L\) (where the equilibrium correlation length \(\xi\) may be arbitrarily large), and metastable stripe states last a finite but large time compared to the coarsening timescale.

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