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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 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 nonconserved scalar fields in two dimensions.

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What is the fate of a kinetic two-dimensional Ising ferromagnet after a quench from above the critical temperature to zero temperature? While the ground state is *always* reached in one dimension and *never* reached in three dimensions [1], the two-dimensional system is enigmatic. Previous numerical evidence indicates that a square lattice system can either get trapped in an infinitely long-lived metastable stripe state with probability close to $\frac{1}{3}$ [1–3] or reach the ground state. In this work, we propose an exact value for the probability for the two-dimensional system to reach the stripe state, thereby establishing that the ground state is not necessarily reached.

Our argument is based on relating the *nonequilibrium* phenomenon of coarsening and *equilibrium* continuum percolation at the critical point. We will exploit this unexpected relation to argue that the probability to reach a stripe state equals $\frac{1}{2}-\frac{\sqrt{3}}{2\pi}\ln\frac{27}{16}=0.3558\ldots$ for free boundary conditions; the corresponding freezing probability for periodic boundary conditions is 0.3390…. This result applies to *any* curvature-driven coarsening process with a nonconserved scalar order parameter, such as the time-dependent Ginzburg-Landau equation [4–6].

Our approach is based on two key observations:

(i) Soon after the quench, an emergent characteristic domain length scale ℓ becomes substantially larger than the lattice spacing a, while remaining much less than the system size L: $a \ll \ell \ll L$. In this regime, this domain mosaic is a realization of the *critical point of continuum percolation*, as previously observed in various two-dimensional systems [7,8] and as argued below.

(ii) In the coarsening regime, $\ell(t) \gg a$, the dynamics becomes deterministic and domain wall evolution is driven only by local curvature [4–6]. Thus the global domain topology does not change once the coarsening regime is reached [9].

These two features imply that the ultimate fate of the system is predetermined 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 *necessarily* reached. Figure 1 shows such 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.

The connection (i) with critical percolation may seem surprising since the initial fraction of spins of a given sign approaches $\frac{1}{2}$ in the large-size limit. This value is below the random site percolation threshold $p_c \approx 0.5927$ on the square lattice. However, after a quench to zero temperature, the spin system quickly approaches the critical state of *continuum* percolation [7]. To appreciate this connection, note that in the coarsening regime (at least the first two panels of Fig. 1), the concentrations of up and down spins remain very close to $\frac{1}{2}$ and the boundaries between spin-up and spin-down domains are smooth and do not contain singular points where four domains meet (as in Fig. 2). This topology coincides with continuum percolation at its threshold; for example, by a surface whose height $\phi(x,y)$ is a random function of (x,y) that is symmetric about $\phi=0$. The regions with positive and negative ϕ correspond to the spin-up and spin-down domains in coarsening, respectively.

While individually observations (i) and (ii) are known, their combined use allows us to apply exact results about crossing probabilities in percolation to determine the final state of the kinetic Ising system in two dimensions. 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 $\mathcal{F}$ and $\mathcal{P}$, respectively. For a critical rectangular system with aspect ratio r (ratio of height to width) [10], the crossing probabilities are nontrivial (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 [13–16], and some of them have been proved in Refs. [17–19].

We begin with the analytically simpler case of free 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, $\mathcal{F}_{\bar{h}v}$, $\mathcal{F}_{h\bar{v}}$, $\mathcal{F}_{hv}$, and $\mathcal{F}_{hv}$ (the dual spanning and non-spanning probabilities are identical by up-down symmetry) therefore satisfy the normalization condition

$$\mathcal{F}_{\bar{h}v} + \mathcal{F}_{h\bar{v}} + 2\mathcal{F}_{hv} = 1. \tag{1}$$

Moreover, the exact form of $\mathcal{F}_{\bar{h}v}$ is known to be [15,16]

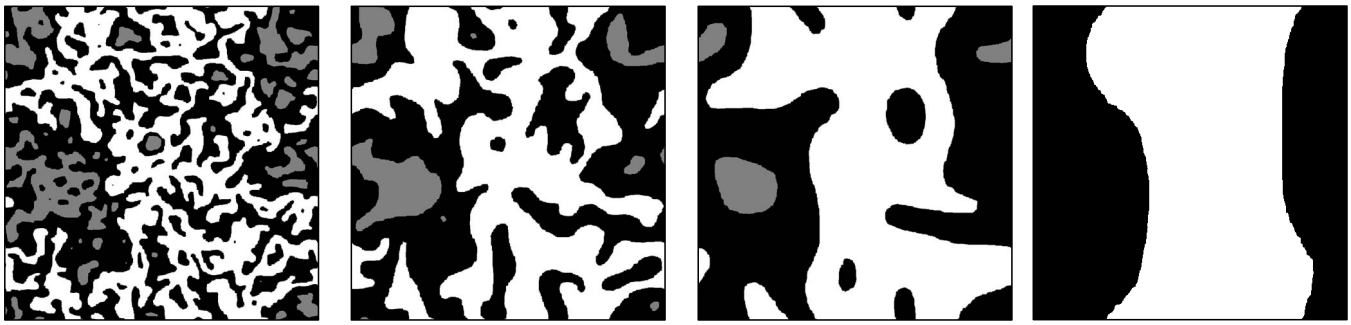

FIG. 1. Coarsening in the kinetic Ising model on a 1024×1024 square lattice with periodic boundary conditions at times (a) 200, (b) 1000, (c) 5000, and (d) 2.5×10^4 Monte Carlo steps following a quench from $T=\infty$ to 0. Domains are regions of either spin up (gray) or spin down (black). A spanning spin-up domain that eventually coarsens into a vertical stripe is highlighted.

$$\mathcal{F}_{\bar{h}v}(r)=\frac{\sqrt{3}}{2\pi}\lambda\,{}_3F_2\left(1,1,\frac{4}{3};\frac{5}{3},2;\lambda\right), \tag{2}$$

where ${}_pF_q(a_1,\ldots,a_p;b_1,\ldots,b_q;\lambda)$ is the generalized hypergeometric function [20], $\lambda=\lambda(r)$ is defined implicitly by

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

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

The corresponding horizontal crossing probability follows by symmetry

$$\mathcal{F}_{h\bar{v}}(1/r)=\mathcal{F}_{\bar{h}v}(r). \tag{3}$$

while the crossing probability for dual spanning satisfies

$$\mathcal{F}_{hv}(r)=\frac{1}{2}[1-\mathcal{F}_{\bar{h}v}(r)-\mathcal{F}_{h\bar{v}}(r)]=\mathcal{F}_{hv}(1/r). \tag{4}$$

The basic relation between Ising domains and critical percolation implies that, e.g., the crossing probability $\mathcal{F}_{\bar{h}v}$ 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.

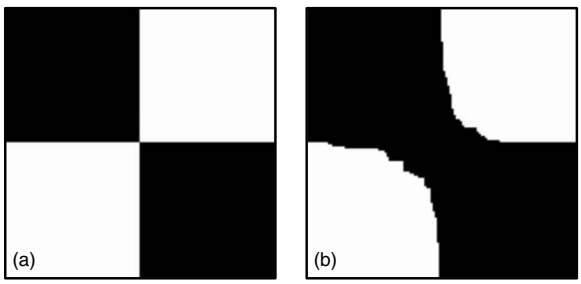

FIG. 2. (a) A state where four Ising domains meet at a single point is dynamically unstable and evolves into (b) a state with no singularities on the domain boundaries.

We simulate many quenches from $T=\infty$ to 0 on lattices of dimension $(256/r)\times256$. For each value of r, we performed 2×10^4 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 simulation results for the probability for a specified ultimate fate of an Ising system with free boundary conditions for a variety of aspect ratios r. The measurements, labeled using the notation $\hat{\mathcal{F}}_{(\ldots)}$, agree well with the corresponding exact crossing probabilities given in Eqs. (2)–(4). For the important special case of a square geometry, $r=1$, Eq. (2) can be simplified to [22],

$$\mathcal{F}_{\bar{h}v}(1)=\mathcal{F}_{h\bar{v}}(1)=\frac{1}{4}-\frac{\sqrt{3}}{4\pi}\ln\frac{27}{16}=0.1779\ldots \tag{5}$$

from which the probability of the Ising system coarsening into a stripe state equals $2\mathcal{F}_{\bar{h}v}(1)=0.3558\ldots$. An earlier numerical estimate for the probability of reaching a stripe state [1] 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 ver-

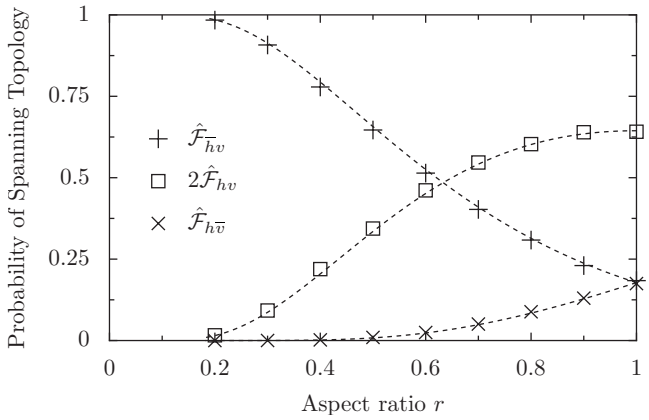

FIG. 3. Probabilities of various domain topologies in the kinetic Ising model following a quench with free boundary conditions: vertical stripes (+), dual-spanning configurations (□), and horizontal stripes (×). Error bars are about 1/3 the symbol size. The lattice dimensions are $(256/r)\times 256$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

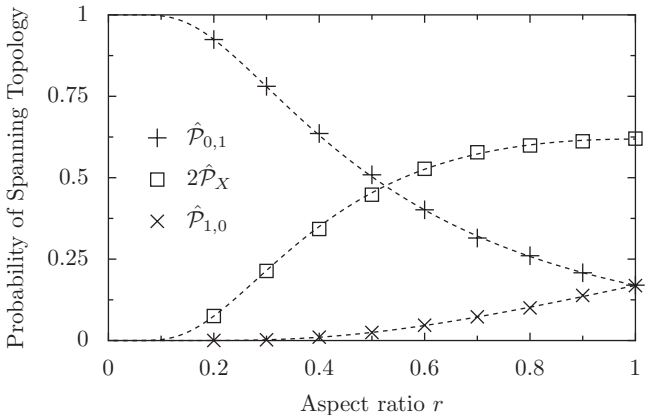

FIG. 4. Probabilities of various domain topologies in the kinetic Ising model following a quench with periodic boundary conditions: vertical stripes (+), dual-spanning configurations (□), and horizontal stripes (×), with error bars about 1/3 of the symbol size. The lattice dimensions are $(256/r)\times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

tical 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 unrolled 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 $\mathcal{P}_{a,b}(r)$ 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]

$$\mathcal{P}_{a,b}(r) = \sum_{l\in\mathbb{Z}} \left[Z_{3al,3bl} - Z_{2al,2bl} - \frac{1}{2} Z_{(3l+1)a,(3l+1)b} - \frac{1}{2} Z_{(3l+2)a,(3l+2)b} + Z_{(2l+1)a,(2l+1)b} \right], \tag{6}$$

where $Z_{m,n}$ is a shorthand for $Z_{m,n}(\frac{2}{3};r)$; generally

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

and $\eta(q)=q^{1/24}\Pi_{k\geq 1}(1-q^k)$ is the Dedekind η function [20]. Additionally, the configuration with cross topology occurs with probability [14]

$$\mathcal{P}_X(r) = \frac{1}{2}\left[Z\left(\frac{8}{3},1;r\right) - Z\left(\frac{8}{3},\frac{1}{2};r\right) \right], \tag{7}$$

where $Z(g,f;r)=f\Sigma_{m,n\in\mathbb{Z}} Z_{fm,fn}(g;r)$. By symmetry, $\mathcal{P}_X(r)$ 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]

$$\mathcal{P}_{0,1}(r) = 1 - 2\rho^{5/4} + \rho^3 + 2\rho^{12} - 4\rho^{53/4} + 3\rho^{15} + \cdots,$$

$$\mathcal{P}_{1,0}(r) = \sqrt{\frac{2r}{3}}(\rho^3 - \rho^{15} - \rho^{27} + 4\rho^{35} + \cdots),$$

$$\mathcal{P}_X(r) = \rho^{5/4} - \rho^3 - 2\rho^{12} + 2\rho^{53/6} - 2\rho^{15} + \cdots,$$

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].

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 $2\mathcal{P}_X$ 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 nonzero 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 $\mathcal{O}(L^2)$.

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…. Because the kinetic Ising model can also evolve to diagonal stripe topologies, $\mathcal{P}_{0,1}+\mathcal{P}_{1,0}+2\mathcal{P}_X$ is less than 1.

In conclusion, the probabilities with which Ising ferro-

magnets freeze into metastable stripe states correspond exactly to crossing probabilities in critical continuum percolation. This correspondence relies on the initial statistical symmetry between up and down spins, which applies when the system is quenched from equilibrium at *any* supercritical initial temperature, $T > T_c$. Our simulation results for the probabilities to reach a specified ultimate fate (Figs. 3 and 4) are in excellent agreement with theoretical predictions. Our approach can be applied 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.

Our theory generally applies to phase ordering kinetics in two dimensions with nonconserved scalar order parameter, as well as to quenches to nonzero subcritical temperatures. In the latter case, the coarsening regime requires that $\xi \ll \ell(t) \ll L$ (where the equilibrium correlation length ξ may be arbitrarily large). Metastable stripe states will now persist for a finite but very long time compared to the coarsening time scale before the final approach to the equilibrium state.

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