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Fate of 2D Kinetic Ferromagnets and Critical Percolation Crossing Probabilities

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We present evidence for a deep connection between the zero-temperature coarsening of both the two-dimensional time-dependent Ginzburg-Landau (TDGL) equation and the kinetic Ising model (KIM) with critical continuum percolation. In addition to reaching the ground state, the TDGL and KIM can fall into a variety of topologically distinct metastable stripe states. The probability to reach a stripe state that winds a times horizontally and b times vertically on a square lattice with periodic boundary conditions equals the corresponding exactly-solved critical percolation crossing probability $\mathcal{P}_{a,b}$ for a spanning path with winding numbers a and b .

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When a ferromagnet with non-conserved spin flip dynamics is quenched from above the critical temperature to zero temperature, a beautiful coarsening domain mosaic emerges [1–3] (Fig. 1). For finite systems, this coarsening ends when the typical domain length reaches the linear dimension of the system. What is the resulting final state? A naive expectation is that the ground state is ultimately reached because each microscopic spin update either decreases or maintains the energy of the system. However, this lowest-energy state is not necessarily the final outcome. There exist a plethora of metastable states, such as straight stripes in two dimensions [4–6] and more bizarre gyroid or “plumber’s nightmare” states in three dimensions [7], which are infinitely long lived at zero temperature. Once the system falls into such a state, the only escape route is via energy-raising spin flips. Since such events do not occur at zero temperature, there is no escape to the ground state.

In the intermediate-time regime, where the typical domain size substantially exceeds the lattice spacing but is much smaller than the system size, the domain mosaic visually resembles the cluster geometry of continuum percolation [8]. This correspondence has sparked recent work on possible connections between these seemingly disparate models [8, 9]. In two dimensions, continuum percolation is critical when the concentrations of both phases are equal [10]. This duality explains why the ground state corresponding to the majority phase is always reached in coarsening in the thermodynamic limit for non-zero initial magnetization [4]. In this case, the majority phase percolates in all directions and inevitably engulfs the entire system. The most interesting situation of quenching from above the critical temperature corresponds to zero initial magnetization, so that the system in the intermediate-time regime is at the critical point of two-dimensional continuum percolation.

The connection to critical percolation is extraordinarily fruitful because it allows us to understand why the system may fall into stripe states rather than ground states and it also predicts the probabilities of various outcomes [8]. For example, the probability to reach a state with vertical stripes [11] equals the spanning prob-

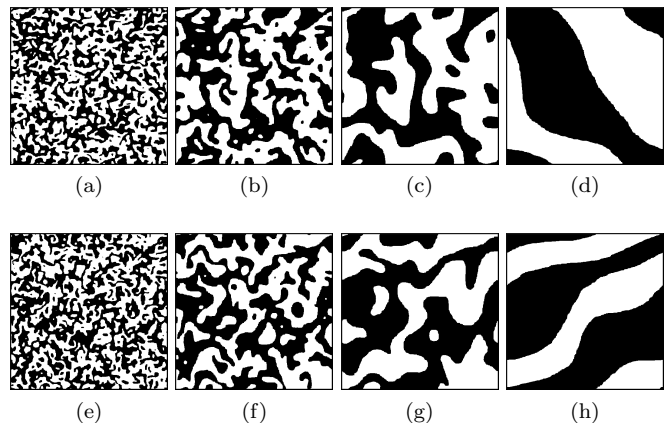


FIG. 1: Snapshots of coarsening in the nearest-neighbor kinetic Ising model on a 1024×1024 square lattice with periodic boundary conditions at: (a,e) $t = 200$, (b,f) 1000, (c,g) 5000, and (d,h) 50000 after a quench from $T = \infty$ to $T = 0$. Top: evolution to $(1, 1)$ stripes (probability ≈ 0.04); bottom: evolution to $(2, 1)$ stripes (probability ≈ 0.00015).

ability $\mathcal{P}_{0,1}$ to have a path that spans the system in the vertical direction at the percolation threshold (and no spanning paths in other directions). The spanning probabilities $\mathcal{P}_{0,1}$ and $\mathcal{P}_{1,0}$ are exactly known [12–14], and this led to the prediction that the probability to reach a stripe state equals $0.3390\dots$ for the square with periodic boundary conditions, in agreement with numerical simulations [8]. (For free boundary conditions this probability is $\frac{1}{2} - \frac{\sqrt{3}}{2\pi} \ln \frac{27}{16} = 0.3558\dots$).

Here we argue that the connection to percolation is much deeper and applies to a large family of positive-energy metastable states, of which straight stripes are merely the simplest members. This connection also applies to a broad class of coarsening models with non-conserved order-parameter dynamics, including the time-dependent Ginzburg-Landau equation (TDGL) [1–3] and the kinetic Ising model (KIM). We will apply the connection to percolation to determine the probabilities to reach general stripe states that wind a times in one Cartesian direction and b times in the orthogonal direction for

both the two-dimensional TDGL and KIM with periodic boundary conditions.

The TDGL for a coarse-grained magnetization density $m(\mathbf{r})$ evolves according to

$$\frac{\partial m}{\partial t} = \nabla^2 m - V'(m), \quad (1)$$

where $V(m) = \frac{1}{2}(1 - m^2)^2$ is the classic double-well potential with minima at $m = \pm 1$ to account for the equilibrium magnetization of a ferromagnetic system. To investigate coarsening that is driven by this TDGL, we discretize this equation and integrate it forward in time by an explicit scheme and average results over many zero-magnetization initial conditions.

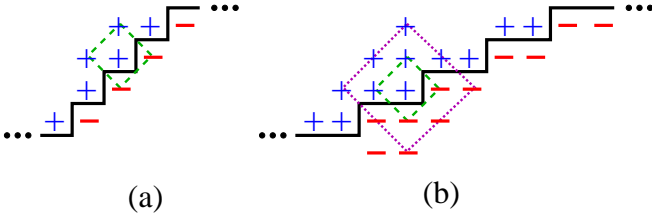


FIG. 2: (a) $[1, 1]^\infty$ staircase interface. With nearest-neighbor interactions (dashed square) interfacial spins can flip freely, but are stable with longer-range interactions. (b) $[2, 1]^\infty$ staircase. Interfacial spins can flip freely with Manhattan metric first- and second-neighbor interactions, but are stable with longer-range interactions.

To reveal the connection to percolation for the discrete KIM, it is essential to extend this model to more distant interactions. The Hamiltonian that we study is

$$\mathcal{H} = -\frac{1}{2} \sum_{i;n} J_n s_i s_{i+n}. \quad (2)$$

For a given spin i , the sum is over the n^{th} -nearest neighbors of s_i , where n^{th} -nearest neighbor is defined (for convenience) by the Manhattan metric, in which the distance between $(0, 0)$ and (x, y) is $|x| + |y|$. We endow this Hamiltonian with single spin-flip dynamics [15]. Operationally, we use Glauber dynamics [16]; we pick a spin at random and flip it if this event decreases the energy of the system. If the energy is unchanged by this flip, the event is accepted with probability $\frac{1}{2}$.

On the basis of universality [17], cooperative behavior of a ferromagnet should not fundamentally depend on the interactions as long as they decay rapidly with distance. However, there are subtle but important interaction-range dependent effects that help expose the parallelism between coarsening in the KIM and critical percolation. For the KIM with second-neighbor ferromagnetic interactions of any magnitude, one sees that the regular $[1, 1]^\infty$

staircase shown in Fig. 2 becomes infinitely long lived. That is, there is an energy cost to flip any spin on either side of this staircase. The stability of this diagonal staircase causes a stripe state that winds once around a periodic square (a torus) in both the x - and y -directions to be infinitely long-lived at zero temperature. Similarly, extending the interaction range to third neighbors additionally causes $[2, 1]^\infty$ and $[1, 2]^\infty$ staircases to become infinitely long-lived and thereby stabilize $(2, 1)$ and $(1, 2)$ stripe states (Fig. 1(h)). As the interaction range becomes infinite [18], stripe states with arbitrary integer winding numbers (a, b) are infinitely long-lived in a square system.

To make the quantitative correspondence between coarsening and percolation, we need exact results for spanning probabilities [12, 19–25], particularly for the torus topology [13, 14]. As above, we label spanning clusters by their horizontal and vertical winding numbers, a and b respectively. Unique classes of spanning clusters arise for each pair of values $a, b \neq 0$ in which a and b are co-prime (i.e., a and b have no common divisors). Stripes that are characterized by (a, b) and by $(-a, -b)$ are equivalent and we therefore set $a > 0$.

Let $\mathcal{P}_{a,b}(r)$ be the probability for a spanning cluster in continuum percolation with winding numbers (a, b) on a rectangle with periodic boundary conditions and with aspect ratio $r \equiv L_y/L_x$. Here L_x and L_y are the linear dimensions of the system in the x - and y -directions. For $L_x, L_y \rightarrow \infty$, this spanning probability is known to be [13, 14]

$$\mathcal{P}_{a,b}(r) = \frac{\mathcal{Z}_{a,b}(6; r) - 2\mathcal{Z}_{a,b}(\frac{8}{3}; r) + \mathcal{Z}_{a,b}(\frac{2}{3}; r)}{2[\eta(e^{-2\pi r})]^2}, \quad (3)$$

where $\eta(q) = q^{1/24} \prod_{k \geq 1} (1 - q^k)$ is the Dedekind η function [26] and $\mathcal{Z}_{a,b}(G; r)$ is the infinite sum

$$\mathcal{Z}_{a,b}(G; r) = \sqrt{\frac{G}{r}} \sum_{j=-\infty}^{\infty} \exp \left[-\pi G \left(\frac{a^2}{r} + b^2 r \right) j^2 \right]. \quad (4)$$

We tacitly assume that $r \geq 1$; for $r < 1$, the spanning probabilities can be extracted from the obvious duality relation $\mathcal{P}_{a,b}(r) = \mathcal{P}_{b,a}(\frac{1}{r})$.

We study the simplest crossing probabilities for a square $L \times L$ system: (i) $\mathcal{P}_0 = \mathcal{P}_{0,1} + \mathcal{P}_{1,0} = 2\mathcal{P}_{0,1}$, the probability for a vertical or horizontal stripe, (ii) $\mathcal{P}_1 = \mathcal{P}_{1,1} + \mathcal{P}_{1,-1} = 2\mathcal{P}_{1,1}$, the probability for a stripe in the $(1, 1)$ or $(1, -1)$ directions, and (iii) for $n \geq 2$, we define $\mathcal{P}_n = 4\mathcal{P}_{n,1}$, the probability for a stripe in the 4 distinct $(\pm n, 1)$ and $(\pm 1, n)$ directions. The series in Eq. (4) converges rapidly in j and we also make use of the series representation of the Dedekind η function,

$$[\eta(\rho^{12})]^{-2} = \rho^{-1} (1 + 2\rho^{12} + 5\rho^{24} + 10\rho^{36} + \dots),$$

with $\rho \equiv e^{-\pi/6}$, to give

$$\begin{aligned}\mathcal{P}_0 &= \sqrt{\frac{8}{3}} \rho^3 (1 - \rho^{12} - \rho^{24} + 4\rho^{32} + \dots) \\ \mathcal{P}_1 &= \sqrt{\frac{8}{3}} \rho^7 (1 + 2\rho^{12} + 2\rho^{24} + 4\rho^{36} + \dots) \\ \mathcal{P}_n &= \sqrt{\frac{32}{3}} \rho^{4n^2+3} (1 + 2\rho^{12} + 5\rho^{24} + 10\rho^{36} + \dots),\end{aligned}\quad (5)$$

where the last line holds for all $n \geq 2$. These stripe probabilities are given to 4-digit accuracy in Table I. Our numerical data for the first three probabilities (Fig. 3), which are practically accessible by simulations, are obtained by a cluster multilabeling method [27]. The extremely good agreement between theory and the simulation results for both the TDGL and the KIM provides strong evidence that there is indeed an intimate connection between percolation crossing probabilities and two-dimensional coarsening.

n	0	1	2	3	4
\mathcal{P}_n	0.3388	0.04196	1.567×10^{-4}	4.438×10^{-9}	1.906×10^{-15}

TABLE I: The probabilities \mathcal{P}_n for $(n, 1)$ stripes on a square lattice for small n .

A second natural set of interesting cases are diagonal stripes with tilt angle $\pm 45^\circ$ on an $L \times nL$ rectangle with periodic boundary conditions. Following the same calculational steps as those given previously for the square system, the series representation for the corresponding probability Π_n is given by

$$\Pi_n = \sqrt{\frac{8}{3n}} \rho^{7n} [1 + 2\rho^{12n} + 2\rho^{24n} + \dots], \quad (6)$$

where again $\rho \equiv e^{-\pi/6}$. From this expression, we numerically obtain the values shown in Table II (to 4-digit accuracy). Our simulation data for Π_n for $n = 2$ and $n = 3$ are consistent with the predictions of Table II. For $n \geq 4$, Π_n is so small that is not practical to accurately measure it by simulations.

n	1	2	3	4
Π_n	0.04196	7.567×10^{-4}	1.582×10^{-5}	3.506×10^{-7}

TABLE II: Π_n for diagonal stripes on a $L \times nL$ rectangle.

An intriguing feature of arbitrary (a, b) stripe states for the discrete Ising model is the intricate nature of the staircase interface between stripes when a and b are both large. The boundaries between the stripe states discussed thus far are either perfect straight lines (vertical and horizontal stripes) or a regular staircase that is inclined at 45° (see Fig. 2(a)). Stability with respect to single spin-flip dynamics imposes severe restrictions on

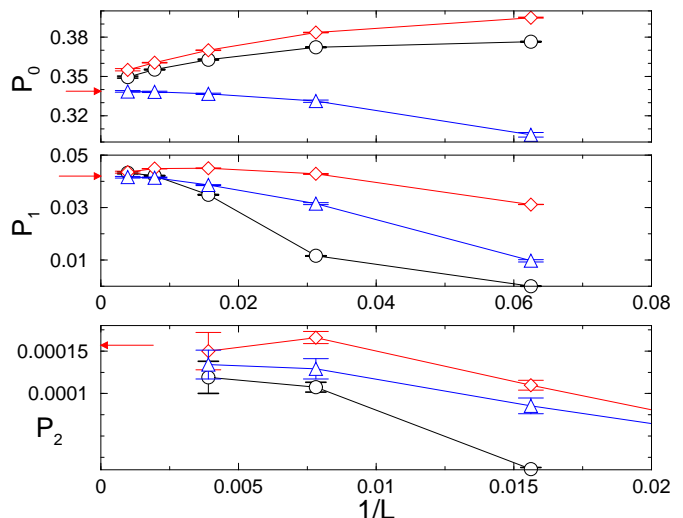


FIG. 3: (a) The stripe probabilities P_0 , P_1 , and P_2 versus $1/L$ for the KIM with nearest-neighbor (\circ) and second-neighbor interactions (\diamond), and for the TDGL (\triangle). Arrows indicate exact values from Table I. For the KIM, data are based on 3.2×10^6 realizations for $L \leq 128$ and 3.2×10^5 realizations for $L = 256$. For the TDGL, data are based on 10^6 realizations for $L \leq 128$ and 5×10^5 realizations for $L = 256$.

the form of these staircases. For example, a stripe with winding numbers $(1, 1)$ could hypothetically arise from a regular staircase that consists of alternating vertical and horizontal steps of length 2. However, such a staircase is unstable because the energy is decreased by flipping the corner spins. This length constraint holds generally: adjacent vertical and horizontal segments in any stable staircase cannot both be longer than 2. Thus the only stable interface for $(1, 1)$ stripes is the regular staircase that we define as $\mathbf{1}^\infty$. This staircase consists of the periodic sequence of building blocks $\mathbf{1} \equiv [1, 1]$, in which $[1, 1]$ denotes a unit-length horizontal segment followed by a unit-length vertical segment.

Continuing this line of reasoning, the only stable staircase in the $(1, n)$ direction is \mathbf{n}^∞ , where $\mathbf{n} = [1, n]$. Similarly, $(\mathbf{12})^\infty$ is the stable staircase in the $(2, 3)$ direction, $(\mathbf{112})^\infty$ is the stable staircase in the $(3, 4)$ direction, $(\mathbf{122})^\infty$ is the stable staircase in the $(3, 5)$ direction, etc. The number of staircases going in the same direction is infinite. For instance, the $(\mathbf{1122})^\infty$ staircase goes in the $(2, 3)$ direction, yet it is unstable. This instability indicates that there is another general rule to build allowed staircase interfaces [28]: only minimal representations are stable. Analysis of stable staircases reveals an intriguing connection with the Farey sequences and the Stern-Brocot tree [29]. To illustrate it, we recall that for two neighbors in some Farey sequence, e.g. for $\frac{1}{2}$ and $\frac{1}{3}$, their ‘sum’ is defined via the rule $\frac{1}{2} \oplus \frac{1}{3} = \frac{1+1}{2+3} = \frac{2}{5}$, and this is taken as an indication that $(\mathbf{23})^\infty$ is the stable staircase in the $(2, 5)$ direction.

The existence of an infinite variety of spanning paths in the KIM with infinite-range interactions also has intriguing implications for the model with short-range interactions. Consider first the classic case of nearest-neighbor interactions. A useful diagnostic to detect metastable stripes with winding numbers $a, b \geq 1$ is to monitor the “survival probability” $S(t)$, defined as the probability that there still exist flippable spins in the system at time t (the term flippable means that when such a spin is flipped, the energy of the system either decreases or remains constant). If there is a single coarsening time τ that scales as L^2 , then one naturally expects that $S(t)$ should asymptotically decay as $e^{-t/\tau}$.

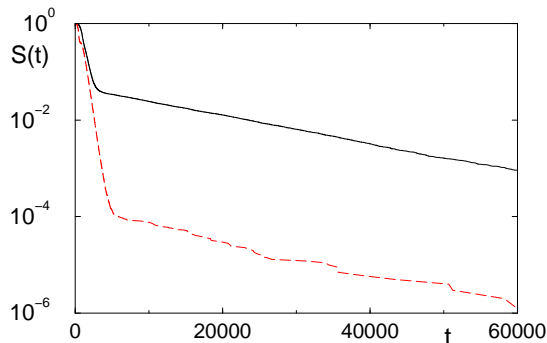


FIG. 4: Survival probability $S(t)$ versus t for the KIM on a 64×64 torus with nearest-neighbor interactions (solid) and second-neighbor interactions (dashed).

The actual behavior is markedly different (Fig. 4), with the evolution of $S(t)$ governed by two time scales [4]. The expected behavior where $S(t) \sim e^{-t/\tau}$ holds until $S(t) \approx 0.05$. At this point, the remaining configurations predominantly have a $(1, 1)$ stripe topology (top line of Fig. 1). As indicated in Fig. 2(a) many of the spins along the interface that separates two diagonal stripes are in zero-energy environments and can flip with no energy cost. The fluctuations of these freely-flippable spins lead to bulk diffusive motion for the interface. When two such diffusing interfaces meet, energy-lowering spin flips occur that ultimately lead the system to the ground state. The decay of $S(t)$ in this asymptotic regime is again exponential in time, but now with characteristic decay time that scales as L^3 [4].

For the KIM with (weaker) second-neighbor ferromagnetic interactions, the vertical and horizontal stripe states, as well as the 1^∞ staircase, are all stable at zero temperature in a square system. Thus at long times, any remaining metastable states are stripes with still higher winding numbers. This feature is reflected in the time dependence of $S(t)$. The decay of $S(t)$ in the second-neighbor KIM is qualitatively similar to that of the nearest-neighbor model, but the break in the decay

now occurs when $S(t) \approx 10^{-4}$ (Fig. 4). The long-lived states that remain beyond this break are predominantly those with winding numbers $(2, 1)$ and $(1, 2)$ that ultimately relax to the ground state by interface diffusion. Such stripe states occur with probability 1.567×10^{-4} (Table I), consistent with the location in the break in the time dependence $S(t)$. While these types of tilted stripe states are ephemeral when the interaction range is finite (albeit with a lifetime that grows as L^3), they become permanent when the interaction range becomes long-ranged.

To summarize, we have presented evidence for a close connection between zero-temperature coarsening of two-dimensional ferromagnets with arbitrary-range but decaying interactions and critical percolation. This connection appears to transcend specific models, as our findings apply equally well to the time-dependent Ginzburg-Landau equation and to discrete kinetic Ising models. The probabilities for either system to evolve to a state that contains stripe paths with specified winding numbers apparently coincides with the exactly-known spanning probabilities in two-dimensional critical percolation. This equivalence suggests that the domain geometry of the kinetic ferromagnets coincides with that of continuum percolation at the critical point.

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