Fate of 2D Kinetic Ising Ferromagnets and Critical Percolation Crossing Probabilities

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We present evidence for a deep connection between the zero-temperature coarsening of the two-dimensional kinetic Ising model (KIM) and critical continuum percolation. In addition to reaching the ground state, the KIM can also 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 an Ising 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 of the kinetic Ising model (KIM) 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, it is now appreciated that 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 the thermodynamic limit) whenever the initial magnetization is non-zero [4]. In this case, the majority phase percolates in all directions and inevitably engulfs the entire system. The most interesting case 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 (in the final state these stripes are straight and have widths ≥ 2) equals the spanning probability $\mathcal{P}_{0,1}$ 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 [11–13], and this led to the prediction that the probability to reach a stripe state equals $0.3390\ldots$ for the square with periodic boundary conditions, in agreement with numerical simulations [8]. (For free boundary conditions this probability is $\frac{1}{2} - \frac{\sqrt{3}}{2\pi} \ln \frac{27}{16} = 0.3558\ldots$).

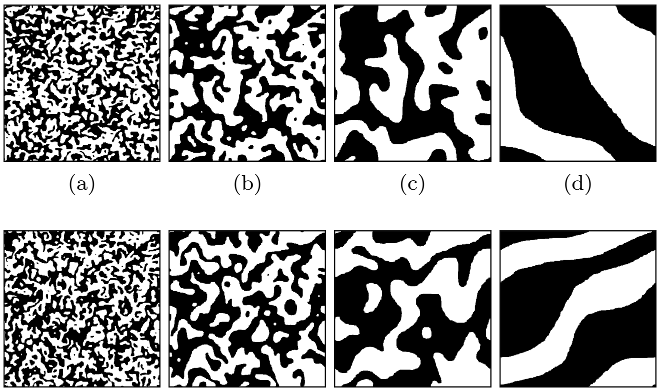
(a) (b) (c) (d)
(e) (f) (g) (h)

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).

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. 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 the two-dimensional KIM with periodic boundary conditions.

To reveal this connection to percolation, it is essential to extend the KIM to more distant interactions. On the basis of universality [14], the dynamical behavior should not depend on the interaction range in a fundamental way. However, there are subtle but important interaction-range dependent effects that help expose the parallelism between coarsening and critical percolation. For convenience, we define range in terms of the Manhattan metric, in which the distance between $(0,0)$ and (x,y) is $|x|+|y|$. By extending the KIM to weaker second-neighbor ferromagnetic interactions, one sees that the regular $[1,1]^\infty$ staircase shown in Fig. 2 become 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 the periodic square (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 the $[2,1]^\infty$ and $[1,2]^\infty$ stripe states to become infinitely long-lived (Fig. 1(h)). As the interaction range becomes infinite [15], stripe states with arbitrary integer winding numbers (a,b) are infinitely long-lived in a square system.

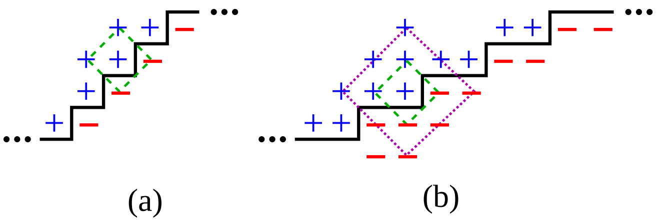

FIG. 2: (a) $[1,1]^\infty$ staircase interface. With nearest-neighbor interactions (dashed square) interfacial spins can flip freely, but are stable with longer-range interactions. (b) $[2,1]^\infty$ staircase. Interfacial spins can flip freely with (Manhattan) first- and second-neighbor interactions,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

To make the quantitative correspondence between coarsening and percolation, we need to make use of several exact results for the probabilities for spanning clusters with specified topologies on the torus at the percolation threshold [11–13, 16–22]. 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. This spanning probability is known to be [12, 13]

$$\mathcal{P}_{a,b}(r)=\frac{\mathcal{Z}_{a,b}(6;r)-2\mathcal{Z}_{a,b}\left(\frac{8}{3};r\right)+\mathcal{Z}_{a,b}\left(\frac{2}{3};r\right)}{2[\eta(e^{-2\pi r})]^2}\,, \qquad (1)$$

where $\eta(q)=q^{1/24}\prod_{k\geq 1}(1-q^k)$ is the Dedekind η function [23] and $\mathcal{Z}_{a,b}(G;r)$ is the infinite sum

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

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

Let us consider 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. (2) converges rapidly in j and we also make use of the series representation of the Dedekind η function,

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

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

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

where the last line holds for all $n\geq 2$. These stripe probabilities are given to 4-digit accuracy in Table I, and our numerical data for the first three probabilities, which are accessible by simulations, are shown in Fig. 3. The agreement between theory and the simulation results is extremely good.

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

$$\Pi_n=\sqrt{\frac{8}{3n}}\,\rho^{7n}\left[1+2\rho^{12n}+2\rho^{24n}+\ldots\right], \qquad (4)$$

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 our predictions. For $n \geq 4$, $\Pi(n)$ is so small that is not practical to accurately measure it by simulations.

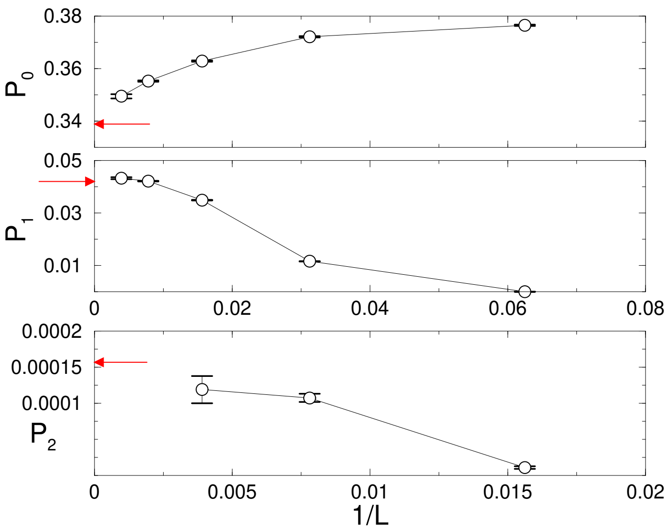

FIG. 3: (a) Numerical values for the stripe probabilities P_0, P_1, and P_2 as a function of $\frac{1}{L}$. The arrows indicate the exact values given in table I.

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 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 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 $\mathbf{n}^\infty$, 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 [25]: only minimal representations are stable. Analysis of stable staircases reveals an intriguing connection with the Farey sequences and the Stern-Brocot tree [24]. 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.

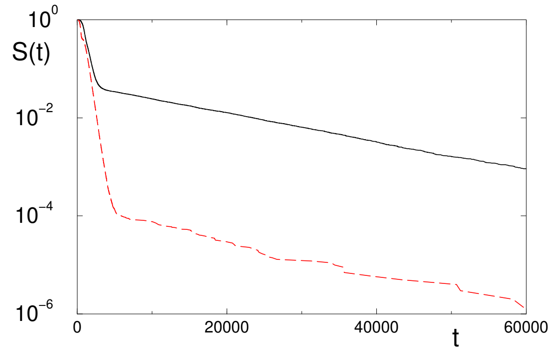

FIG. 4: Survival probability $S(t)$ versus t on a semi-logarithmic scale for the KIM on a 64×64 torus with nearest-neighbor interactions (solid) and second-neighbor interactions (dashed).

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 $e^{-t/\tau}$.

However, 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 $S(t)$ has decayed to approximately 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 staircase $[1,1]^\infty$, 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 the same interface diffusion mechanism as that for the $(1,1)$ winding-number states with nearest-neighbor interactions. The probability for such stripe states to occur was previously found to be 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 (albeit with a lifetime that grows as L^3) when the interaction range is finite, they become permanent when the interaction range becomes long-ranged.

While we have focused exclusively on single spin-flip dynamics, the connection to critical percolation appears to be much more general. We have verified [25] that the same stripe probabilities arise in simulations of the time-dependent Ginzburg-Landau equation [1–3] as in the kinetic Ising model. We therefore anticipate that the connection to percolation will be valid for any curvature-driven coarsening process with a non-conserved scalar order parameter.

To summarize, we have presented evidence for a close connection between zero-temperature coarsening of the kinetic Ising model with arbitrary-range but decaying ferromagnetic interactions and critical percolation. The probabilities for the kinetic Ising 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 Ising model coincides with that of continuum percolation at the critical point.

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