Zero-Temperature Freezing in Three-Dimensional Kinetic Ising Model

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We investigate the long-time properties of the Ising-Glauber model on a periodic cubic lattice after a quench to zero temperature. In contrast to the conventional picture from phase-ordering kinetics, we find: (i) Domains at long time are highly interpenetrating and topologically complex, with average genus growing algebraically with system size. (ii) The long-time state is almost never static, but rather contains "blinker" spins that can flip *ad infinitum* with no energy cost. (iii) The energy relaxation has a complex time dependence with multiple characteristic time scales, the longest of which grows exponentially with system size.

PACS numbers: 64.60.My, 75.40.Gb, 05.50.+q, 05.40.-a

Phase ordering kinetics is concerned with the growth of domains of ordered phase when a system is suddenly cooled from a high-temperature spatially-homogeneous phase to a subcritical temperature [1–3]. For systems with a non-conserved order parameter, single-phase regions emerge and form a coarsening domain mosaic whose typical length scale grows in time as $t^{1/2}$. This growth continues until the system reaches the equilibrium state with a non-zero order parameter. An archetypical example is the Ising model that is endowed with Glauber dynamics [4], where domains consist of contiguous regions of spins that all point up or point down.

What happens when the final temperature is zero? While an infinite system will coarsen indefinitely, coarsening should stop in a finite system of linear dimension L when the typical domain length becomes comparable to L. A natural expectation is that the ground state will ultimately be reached, and indeed this outcome occurs in the one-dimensional Ising-Glauber model [2, 3]. Surprisingly, this conventional picture already begins to fail in two dimensions where the ground state is reached roughly two-thirds of the time; in the remaining cases, the system falls into an infinitely long-lived metastable state that consists of two (and more than two in rare cases) straight single-phase stripes [5–7].

The fate of the three-dimensional Ising ferromagnet with zero-temperature Glauber dynamics is even more intriguing. First, the long-time state is topologically complex, with multiply-connected interpenetrating regions of positive and negative magnetization. This sponge-like geometry represents a discrete analog of zero average-curvature interfaces, for which a veritable zoo of possibilities have been cataloged [8, 9]. There is also a close resemblance to gyroid phases, or "plumber's nightmares" that arise in micellar and other two-phase systems [10–13]. Second, even though the temperature is zero, almost all realizations fluctuate forever due to *blinker spins* — a subset of spins that can flip repeatedly without any energy cost [5]. Last, the approach to these asymptotic blinker states is extraordinarily slow, with relaxation times that grow exponentially with system size. If the initial magnetization is non-zero, it is believed that the ground state of the initial majority phase is reached [5, 14], while if the boundary spins have a fixed sign the ground state is always reached [15].

Our system is the three-dimensional homogeneous ferromagnetic Ising model on a cubic lattice of linear dimension L with periodic boundary conditions. The system is initialized in the antiferromagnetic state [16, 17] and spins subsequently evolve by zero-temperature Glauber dynamics: a randomly-selected spin flips with probability 1 if the energy of the system decreases, flips with probability $\frac{1}{2}$ if the energy does not change, and does not flip if the energy were to increase.

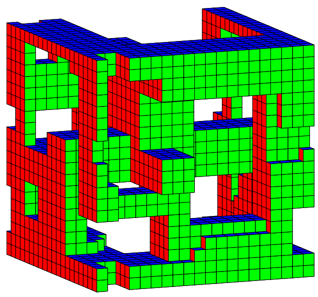

FIG. 1: (color online) Example of a genus $g = 17$ final-state domain on a 20^3 lattice with periodic boundary conditions. Each block represents an up spin (with the spin at the center of the block), while blank space represents a down spin.

`Energy and Topological Complexity:` A fundamental characteristic of the long-time state is the dependence of the energy gap (per spin) E_L versus system size L. Even though the system does not reach the ground state, the energy systematically decreases with L. Direct simulations to reach the asymptotic state of even medium-size systems are prohibitively slow, however, because energy-lowering spin-flip events become progressively more rare once the coarsening length scale reaches the system size. In this post-coarsening regime, the energy evolution is characterized by long periods where only zero-energy spins (those with equal numbers of up and down neighbors) flip, punctuated by rare energy-decreasing events.

To reduce the time needed to simulate these long iso-energy wanderings, we employ an acceleration protocol: Once energy-lowering events become rare, we apply an infinitesimal magnetic field as the system wanders on each energy plateau between energy-lowering events [18]. The field drives the state-space motion on each plateau so that the next energy-lowering spin flip is found more quickly. After each energy-lowering event, the direction of the infinitesimal field is reversed so that the net average field is zero. We verified that this procedure accurately reproduces the energy that is obtained by Glauber dynamics for the range of system sizes ($L \leq 10$) where a direct check of this acceleration method is computationally feasible [17]. (The relative deviation of the average energies obtained by these two approaches is less than 10^{-7} for size 10^3, while taking a factor of 58 less CPU time.)

Our data for the energy is based on systems of linear dimension $L \leq 76$ with $\geq 10^5$ realizations for each value of L. The relative error for each data point is $< 0.1\%$. Our data are consistent with $E_L \sim L^{-\epsilon}$ with $\epsilon \approx 1$, in agreement with previous results based on smaller-scale simulations [5]. This dependence implies that the total interface area between spin domains scales as L^2.

At long times, there are almost always just two interpenetrating domains [17], and these domains are topologically complex. We quantify a domain topology by its genus g, which equals the number of holes in the domain surface. (The genus of a sphere is $g = 0$, while the genus of a doughnut is $g = 1$.) Figure 1 shows a large-genus example (with $g = 17$) for a 20^3 periodic system. To measure the genus of a domain, we exploit the connection to the Euler characteristic [19]

$$\chi = 2(1 - g) = V - E + F \tag{1}$$

that relates χ to easily-measured features of the interface: V, the number of vertices on the interface, E, the number of edges, and F, the number of faces. Each face separates a pair of oppositely-oriented neighboring spins, so that F is directly related to the energy by $F \sim L^3 E_L$. Our simulation data for systems with $L \leq 76$ again show considerable finite-size corrections but extrapolation suggests that the average genus grows as $\langle g\rangle \sim L^\gamma$ with $\gamma \approx 1.7$.

The final energy E_L leads to an upper bound on the genus g. To establish this bound, we simplify Eq. (1) by noting that a face has 4 edges, and each edge is shared between 2 adjacent faces. Hence $E = 2F$. Similarly, each edge has 2 vertices that are shared among 3, 4, or 5 adjacent edges, giving $\frac{2}{5}E \leq V \leq \frac{2}{3}E$. Using these relations in Eq. (1) gives $-\frac{1}{5}F \leq \chi \leq \frac{1}{3}F$, or $0 \leq g \leq 1 + \frac{1}{10}F$ where we additionally use that the number of holes g is non-negative. From the relation between the number of faces and the energy, $F \sim L^3 E_L \sim L^{3-\epsilon}$, with $\epsilon \approx 1$, we have the upper bound $g \leq L^{3-\epsilon}$. This growth rate is slightly faster than that suggested by our simulations, $\langle g\rangle \sim L^\gamma$, with $\gamma \approx 1.7$.

`Blinker States:` As the linear dimension is increased, it becomes overwhelmingly likely that the system does not reach a static state at long times, but rather, gets trapped within a set of perpetually evolving configurations that contain stochastic *blinker* spins. In Fig. 2, spins that point up lie at the center of the small cubes and blinker spins are highlighted, while down spins are represented by blank space. Equivalently, spin-up blinkers are located at the convex (outer) corners of the interface, while spin-down blinkers are adjacent to the apex of the concave (inner) corners. Each blinker spin has three neighboring spins of the same sign and three of the opposite sign so that a blinker can flip without changing the energy of the system. When a blinker spin flips, one of its neighbors typically becomes a blinker so that blinkers never cease to evolve.

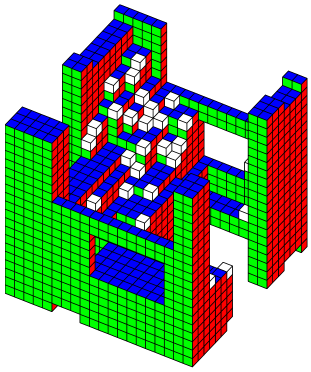

FIG. 2: (color online) An example of a blinker state on a 20^3 cubic lattice with periodic boundary conditions. Highlighted blocks correspond to "blinker" spins that point up.

A system that contains blinker spins can therefore wander forever on a small set of iso-energy points in state space. We define this set as a *blinker state*. While the fraction of blinker spins is small — typically less than a percent when the linear dimension $L \geq 10$ — the fraction of the system volume over which blinker spins can wander is roughly 9% for large L [17].

These blinkers are part of the huge number of metastable states in the system. For example, the number of metastable states that consist of alternating slabs of plus and minus spins (the three-dimensional analog of stripe states in two dimensions) scales as $\exp(L^2)$ [5]; a similar estimate for the number of metastable sponge-like states gives $\exp(L^3)$ [20]. Thus it is plausible that the three-dimensional Ising model with Glauber dynamics should get trapped in one of these ubiquitous metastable states. What is striking, is that the system almost always falls into a perpetually evolving blinker state, rather than a static metastable state. For example, for 10^5 realizations at $L = 76$, the fraction of realizations that end in a blinker state, a static metastable state, and the ground state are 97.46%, 2.50%, and .04%, respectively.

`Ultra-Slow Relaxation:` Blinker states are also responsible for an extremely slow relaxation that involves time scales that grow faster than power law in the system size [21]. To understand the cause of these long time scales, consider the synthetic cubic blinker state shown in Fig. 3. By zero-energy spin flips, the interface defined by the blinker spins can be in the extremes of fully deflated (left), intermediate (middle), or fully inflated (right). Although each blinker spin does not have any energetic bias, there exists an effective geometric bias that drives the interface to the half-inflated state. This effective bias stems from the difference in the number of flippable spins on the convex (outer) and concave (inner) corners on the interface, N_+ and N_-, respectively. When the interface is mostly inflated, $N_+ - N_-$ is positive, so that there are, on average, more spin flip events that tend to deflate the interface, and vice versa when the interface is mostly deflated. This effective bias drives the interface to the half-inflated state.

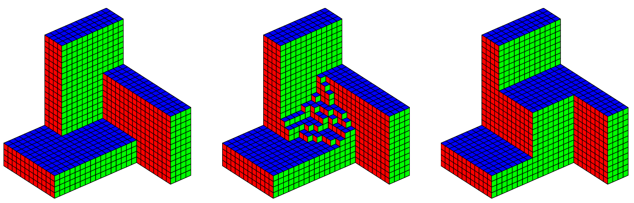

FIG. 3: (color online) An $8\times 8\times 8$ blinker on a 20^3 cubic lattice, showing the fully-deflated (left), intermediate (middle), and fully-inflated states (right). The bounding slabs wrap periodically in all three Cartesian directions.

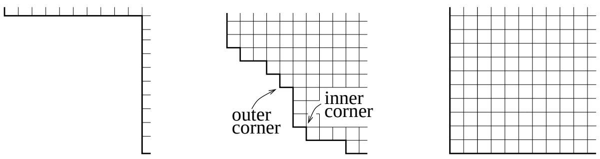

FIG. 4: Two-dimensional analog of the blinker states in Fig. 3.

We quantify the relaxation of this blinker by the first-passage time $\langle t\rangle$ for an $\ell\times\ell\times\ell$ half-inflated blinker (Fig. 3 middle) to reach the fully-inflated state. For simplicity, consider first the corresponding two-dimensional system (Fig. 4). Near the half-inflated state, the interface consists of N_+ outer corners and N_- inner corners, with $N_+ - N_-$ always equal to 1 in two dimensions, and $N_+ \sim \ell$ [22]. In one time unit, all eligible spins on the interface flip once, on average. Since $N_+ - N_- = 1$, the area occupied by the up spins typically decreases by 1. Thus we infer an interface velocity $u = \Delta A/\Delta t \sim -1$. Similarly, since there are $N_+ + N_- \sim N_+$ spin flip events in one time unit, the mean-square change in the interface area is of the order of $N_+ \sim \sqrt{A} \sim \ell$. Thus the effective diffusion coefficient is $D \sim \ell$. The underlying first-passage process from the half-inflated to the fully-inflated state requires moving against the effective bias velocity by flipping $\ell^2/2$ spins to point up. Consequently, the dominant Arrhenius factor in the first-passage time is $\tau \sim \exp(|u|\ell^2/2D)$, so that [23]

$$\ln\tau \sim \ell\,. \tag{2}$$

For the corresponding three-dimensional blinker, the inflated region is a cube of volume ℓ^3. There are typically $N_\pm \sim \ell^2$ outer and inner corners on the interface when it is half inflated. In distinction with two dimensions, there is no conservation law for the difference $N_+ - N_-$. Rather, the disparity between N_+ and N_- is of the order of ℓ. If the system is beyond the half-inflated state, then in a single time step the interface will recede, on average, by ℓ, giving an interface velocity $u \sim \ell$. Similarly we estimate $D \sim N_\pm \sim \ell^2$, leading to

$$\ln\tau \sim u\ell^3/D \sim \ell^2\,. \tag{3}$$

The straightforward generalization to d dimensions gives $\ln\tau \sim \ell^{d-1}$. Our simulations [17] for this first-passage time in two dimensions agree with Eq. (2). In three dimensions, simulations are necessarily limited to small ℓ, while our crude argument is asymptotic. Moreover, the bias velocity in three dimensions is not strictly constant during the inflation of the interface, while the bias is constant in two dimensions. Nevertheless, the meager data that we do have (up to $\ell = 5$) are qualitatively consistent with Eq. (3). The salient result is that the time for a half-inflated blinker to reach the fully-inflated state grows extremely rapidly with ℓ.

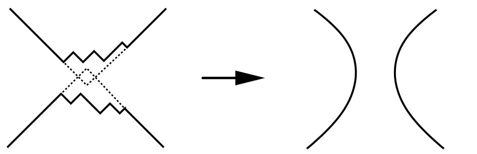

FIG. 5: Two-dimensional sketch of blinker coalescence.

From the dynamics of the cubic blinker of Fig. 3, we can understand the long-time relaxation of a large system. Indeed, suppose that there are two such blinkers that are oppositely oriented and spatially separated so that they do not overlap when both are half inflated, but just touch corner to corner when both are inflated (Fig. 5). As long as the blinkers do not overlap, their fluctuations do not change the energy of the system. However, if these blinkers touch, then a spin flip event has occurred that lowers the energy. After this irreversible coalescence event, subsequent spin flips cause the two blinkers to ultimately merge. Each of these initial coalescences corresponds to one of the increasingly rare energy-lowering spin-flip events at long times.

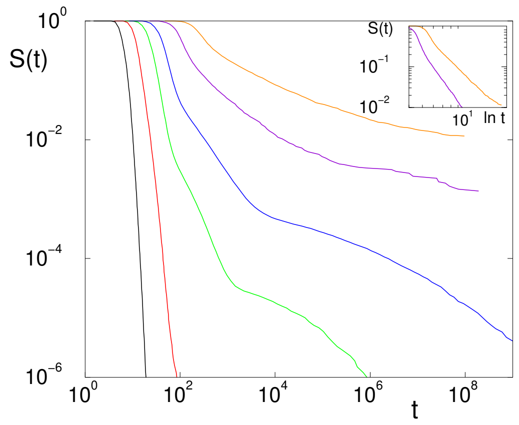

FIG. 6: (color online) Survival probability for $L = 4, 6, 8, 10, 14$ and 20 (lower left to upper right) for 10^7 realizations $L \leq 10$ and 10240 realization for $L = 14$ and 20 on a double logarithmic scale. The inset shows $S(t)$ versus $\ln t$ for $L = 14$ and 20 on a double logarithmic scale.

To quantify this long-time relaxation, we study $S(t)$, the probability that the energy of the system is still decreasing at time t (Fig. 6). In two dimensions, this survival probability decays as $S \sim e^{-t/\tau}$, with a decay time $\tau(L)$ that suddenly changes from a quadratic dependence on L to a faster dependence after $S(t)$ has decayed by roughly two orders of magnitude [5, 24]. This transition is caused by long-lived but finite-lifetime metastable configurations in which the spins organize into two diagonal stripe domains that wind around the torus once in both the toroidal and poloidal axes [5].

The corresponding behavior in three dimensions is more enigmatic and suggests multiple temporal regimes. At short times, $S(t)$ is nearly constant because the coarsening length scale has not yet reached L. Subsequently $S(t)$ first decays rapidly with time, and eventually more slowly. As shown in Fig. 6, nearly 10% of all realizations of a 20^3 system are still evolving at $t = 10^4$ and more than 1% are still evolving at $t = 10^8$, whereas the coarsening time scale is only 400. For the largest systems for which we could simulate $S(t)$ to long times, the decay $S(t)$ seems to reasonably fit an inverse logarithmic law $S(t) \sim (\ln t)^{-1}$ (Fig. 6 inset), a dependence that occurs in simple [21] and glassy spin systems [25], as well as in granular compaction [26].

Thus a basic statistical-mechanics model, the three-dimensional Ising model with zero-temperature Glauber dynamics, does not reach the ground state. The relaxation is extraordinarily slow and almost all realizations eventually reach a blinker state, which is a set of connected iso-energy points in the space of metastable states, where the system wanders forever. Domain interfaces are topologically complex, with hints of a simple relation between the genus of domains and the long-time energy.

We gratefully acknowledge financial support from NSF Grants No. DMR-0906504 (JO and SR).

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