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Zero-temperature freezing in the three-dimensional kinetic Ising model

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We investigate the relaxation 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 the following: (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 is extremely slow, with a characteristic time that grows exponentially with system size.

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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 [1,2]. For systems with a nonconserved order parameter, single-phase regions emerge to 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 nonzero order parameter. An archetypical example is the Ising model endowed with Glauber dynamics [3], 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 might be that the ground state is ultimately reached, and this outcome indeed occurs in the one-dimensional (1D) Ising-Glauber model [1,2]. Surprisingly, the conventional picture already begins to fail in 2D 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 (or more in rare cases) straight single-phase stripes [4–6].

The fate of the 3D Ising ferromagnet with zero-temperature Glauber dynamics is even more intriguing (Fig. 1). First, the long-time state is topologically complex, with multiply connected interpenetrating regions of positive and negative magnetization. This spongelike geometry represents a discrete analog of zero average-curvature interfaces, for which a veritable zoo of possibilities have been cataloged [7,8]. There is also a close resemblance to gyroid phases, or "plumber's nightmares," that arise in micellar and other two-phase systems [9]. 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 [4]. Last, the approach to these asymptotic blinker states is extraordinarily slow, with a relaxation time that grows exponentially with system size. In contrast, if the initial magnetization is nonzero, it is believed that the ground state of the initial majority phase is reached [4,10].

We study the 3D homogeneous Ising ferromagnet on a cubic lattice of linear dimension L with periodic boundary conditions. The spins are initialized in the antiferromagnetic state [11,12] and subsequently evolve by zero-temperature Glauber dynamics: a randomly selected spin flips with probability 1 if the energy decreases, flips with probability $\frac{1}{2}$ if the energy does not change, and does not flip if the energy increases.

I. ENERGY AND TOPOLOGICAL COMPLEXITY

A fundamental characteristic of the long-time state is the dependence of the energy gap (defined as the energy difference about the ground state per spin) E_L versus system size L. Even though the ground state is not reached, 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 fixed-energy plateau between energy-lowering events [13]. 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 spin flip, the direction of the infinitesimal field is reversed so that the net time-average field is zero. We systematically checked that this procedure accurately reproduces the energy that is obtained by Glauber dynamics for system sizes ($L \leqslant 10$) where a direct check of this acceleration method is computationally feasible [12]. We find that the relative difference in the average energies obtained by these two approaches is less than 10^{-7} for size 10^3, while taking two orders of magnitude less CPU time. Our energy data are based on systems of linear dimension $L \leqslant 76$ with $\geqslant 10^5$ realizations for each 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 much smaller-scale simulations [4].

At long times, there are almost always just two interpenetrating and topologically complex domains [12]. We quantify

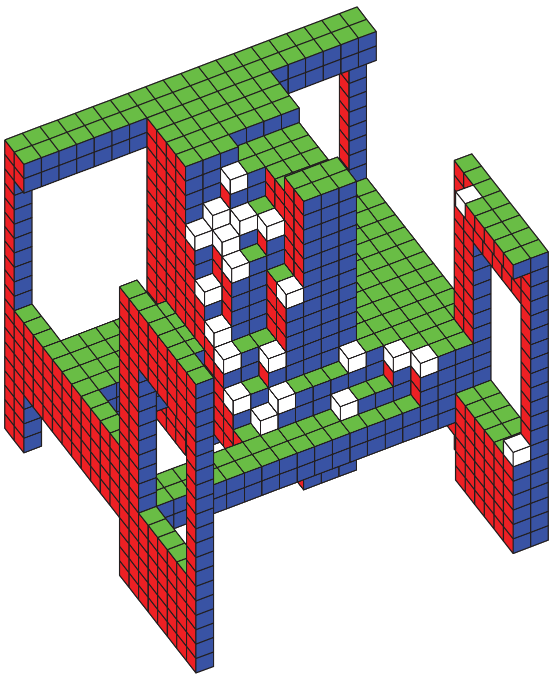

FIG. 1. (Color online) Example of a genus $g = 10$ domain on a 20^3 lattice with periodic boundary conditions. Each block represents an up spin (with the spin at the center of the block), while blank space represents a down spin. Highlighted blocks correspond to "blinker" spins (see text) that point up.

domain topology by the genus g, which equals the number of holes in the domain surface. (For example, the genus of a sphere is $g = 0$, while that of a doughnut is $g = 1$.) Figure 1 shows an example with $g = 10$ for a 20^3 periodic system. To measure the domain genus, we exploit the connection to the Euler characteristic [14],

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

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

A simple topological argument relates the average final energy E_L and average genus $\langle g \rangle$. To establish this relation, we simplify Eq. (1) by noting that a face has four edges, and each edge is shared between two adjacent faces. Hence $\mathcal{E} = 2\mathcal{F}$ [14]. Similarly, each edge has two vertices that are shared among three, four, five, or six adjacent edges, giving $\frac{1}{3}\mathcal{E} \leqslant \mathcal{V} \leqslant \frac{2}{3}\mathcal{E}$. Using these relations in Eq. (1) gives $-\frac{1}{3}\mathcal{F} \leqslant \chi \leqslant \frac{1}{3}\mathcal{F}$, or $0 \leqslant g \leqslant 1 + \frac{1}{6}\mathcal{F}$, where we also use that the number of holes (the genus) is non-negative. Since $\mathcal{F} \sim L^3 E_L \sim L^{3-\epsilon}$ with $\epsilon \approx 1$, we therefore obtain the upper bound $g \leqslant L^{3-\epsilon}$, or equivalently, the fundamental exponent relation $\epsilon + \gamma \leqslant 3$. Our simulational estimates for these two exponents $\epsilon \approx 1$ and $\gamma \approx 1.7$ indicate that this bound is numerically meaningful.

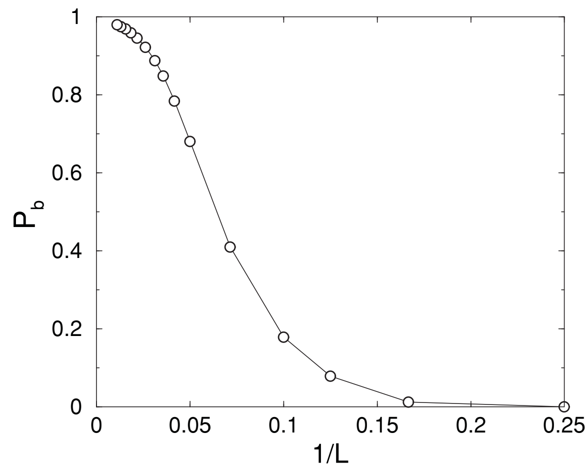

FIG. 2. Plot of P_b, the probability of reaching a blinker configuration as a function of $1/L$.

II. BLINKER STATES

As the linear dimension is increased, the system almost always (Fig. 2) gets trapped within a set of perpetually evolving configurations that contain stochastic *blinker* spins. 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 (see Fig. 1). Equivalently, spin-up blinkers exist at convex (outer) corners of domain interfaces, while spin-down blinkers are adjacent to the apex of concave (inner) corners. When a blinker spin flips, one (or more) of its neighbors typically becomes a blinker so that these configurations never cease to evolve.

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 $L \geqslant 10$—the fraction of the system volume over which blinker spins can wander is roughly 9% for large L [12].

These blinkers are part of a huge number of spongelike metastable states in the system whose number is estimated to scale as $\exp(L^3)$ [15]. [These states are much richer in character that the alternating-stripe metastable states in 2D, whose number grows as λ^L, where $\lambda = \frac{1}{2}(1 + \sqrt{5})$ is the golden ratio [4].] Thus it is plausible that the 3D Ising model with Glauber dynamics should get trapped in one of these ubiquitous metastable states. What is unexpected is that the system almost always falls into a perpetually evolving blinker state rather than a static metastable state. For example, for $L = 76$, 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 (Fig. 2).

III. ULTRASLOW RELAXATION

Blinker states are responsible for an extremely slow relaxation whose time scale grows faster than a power law in the system size [16]. To understand the cause of this long time scale, consider the synthetic blinker shown in Fig. 3. By zero-energy spin flips, the interface defined by the blinker spins can be fully deflated (left), partially inflated (middle), or

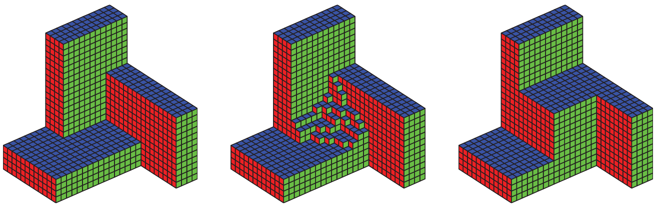

FIG. 3. (Color online) An $8 \times 8 \times 8$ blinker on a 20^3 cubic lattice, showing the fully deflated (left), partially inflated (middle), and fully inflated states (right). The bounding slabs wrap periodically in all three Cartesian directions.

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 typically 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.

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 2D system (Fig. 4). Near the fully inflated state, the interface consists of N_+ outer corners and N_- inner corners, with $N_+ - N_-$ always equal to 1 in 2D, and $N_+ \sim \ell$ [17]. 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 that keeps the blinker near half-inflation by flipping $\ell^2/2$ spins. Consequently, the dominant Arrhenius factor in the first-passage time is $\tau \sim \exp(|u|\ell^2/2D)$, so that $\ln \tau \sim \ell$ [18].

For the corresponding 3D 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 contrast to 2D, 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 blinker is beyond half-inflation, 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 $\ln \tau \sim u\ell^3/D \sim \ell^2$. The straightforward generalization to d dimensions gives $\ln \tau \sim \ell^{d-1}$. Our simulations [12] for this first-passage time in 2D agree with $\ln \tau \sim \ell$. In 3D, simulations are necessarily limited to small ℓ, while our crude argument is asymptotic. Moreover, the bias velocity in 3D is not strictly constant during the inflation of the interface, while the bias is constant in 2D. Nevertheless, the meager data that we do have (up to $\ell = 5$) are qualitatively consistent with $\ln \tau \sim \ell^2$. The salient result is that the time for a half-inflated blinker to reach full inflation grows extremely rapidly with ℓ.

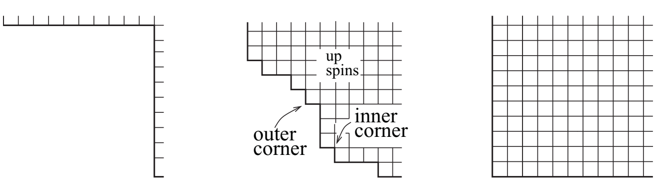

FIG. 4. Two-dimensional analog of the blinker states in Fig. 3.

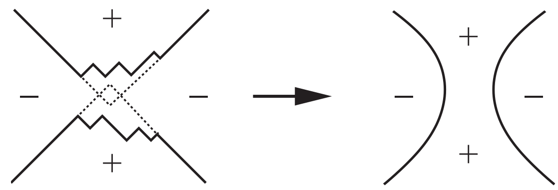

FIG. 5. Two-dimensional sketch of blinker coalescence.

The dynamics of the cubic blinker of Fig. 3 helps us to 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 deflated, 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, when these blinkers touch, then a spin-flip event has occurred that lowers the energy. Each such event corresponds to one of the increasingly rare energy-lowering spin-flip events at long times. Subsequent spin flips then cause the two blinkers to ultimately merge.

To describe the relaxation of the Ising ferromagnet, we study $S(t)$, the probability that the energy of the system is still decreasing at time t (Fig. 6). In 2D, this survival probability can be represented as a sum of two exponential decays with very different decay times, the longer of which arises from diagonal stripe domains [4]. The corresponding relaxation in 3D is much slower and much harder to quantify. In fact, we observe that the energy is still decreasing at $t = 10^4$ in nearly 10% of all realizations of a 20^3 system, and is still decreasing in more

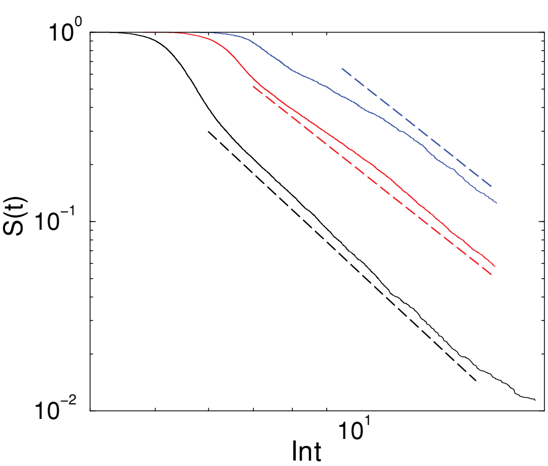

FIG. 6. (Color online) Double logarithmic plot of $S(t)$ vs $\ln t$ for $L = 20$, 30 (10 240 realizations) and 40 (2048 realizations) from lower left to upper right. The lines are guides to the eye, with slopes 3.3, 2.8, and 2.8 for $L = 20$, 30, and 40.

than 1% of all realizations at $t = 10^8$, whereas the coarsening time scale is only 400. Our data suggest that $S(t)$ decays as $(\ln t)^{-\psi}$, with $\psi \approx 3$ (Fig. 6), an unusual time dependence that also occurs in homogeneous [16] and glassy spin systems [19], as well as in granular compaction [20].

To summarize, a basic statistical-mechanical model, the 3D Ising model with zero-temperature Glauber dynamics, reaches a topologically complex long-time state. By using elementary topological arguments, we showed that the genus of the domains and the long-time energy of the system are simply interrelated. We believe that ideas from topology will prove useful for discovering many more striking topological properties of domains. The energy relaxation is extraordinarily slow and almost all realizations eventually reach a blinker state—a set of connected iso-energy points in the space of metastable states, where the system wanders forever. These blinker states are surprisingly ubiquitous, as nearly every realization ends in a blinker state. The time scale associated with the relaxation of the blinker states scales exponentially with the system size; this is many orders of magnitude longer than the coarsening time, which scales as L^2. We anticipate that many surprising properties will also arise in the zero-temperature coarsening in noncubic geometries and in models with a higher-dimensional order parameter.

ACKNOWLEDGMENTS

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