Fate of zero-temperature Ising ferromagnets

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We investigate the relaxation of homogeneous Ising ferromagnets on finite lattices with zero-temperature spin-flip dynamics. On the square lattice, a frozen two-stripe state is apparently reached approximately 3/10 of the time, while the ground state is reached otherwise. The asymptotic relaxation is characterized by two distinct time scales with the longer stemming from the influence of a long-lived diagonal stripe defect. In greater than two dimensions, the probability to reach the ground state rapidly vanishes as the size increases and the system typically ends up wandering forever within an iso-energy set of stochastically ''blinking'' metastable states.

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What happens when an Ising ferromagnet, with spins endowed with Glauber dynamics [1], is suddenly cooled from a high temperature to zero temperature ($T=0$)? A first expectation is that the system should coarsen [2] and eventually reach the ground state. However, even the simple Ising ferromagnet has a large number of metastable states with respect to Glauber spin-flip dynamics. Therefore at zero temperature the system could get stuck forever in one of these states.

In this paper, we argue that the kinetics of this system is richer than either of these scenarios. While the ground state is always reached in one dimension, there appears to be a nonzero probability that the square lattice system freezes into a stripe configuration for equal initial densities of ↑ and ↓ spins [3]. The relaxation is governed by two distinct time scales, the larger of which stems from a long-lived diagonal stripe defect. On hypercubic lattices ($d\geqslant 3$), the probability to reach the ground state vanishes in the thermodynamic limit and the system wanders forever on an isoenergy subset of connected metastable states. Again, the relaxation seems to be characterized by at least two time scales.

It bears emphasizing that these long-time anomalies require that the limit $T\rightarrow 0$ is taken *before* the thermodynamic limit $L\rightarrow\infty$. Very different behavior occurs if $L\rightarrow\infty$ before $T\rightarrow 0$ [4]; a system that enters a metastable state can escape and the true equilibrium state is eventually reached. However, for $T=0$, a system which enters a metastable state will be trapped forever.

We can easily appreciate the peculiarities of zero-temperature dynamics for odd-coordinated lattices such as the honeycomb lattice. Here a connected cluster in which each spin has at least two aligned neighbors is energetically stable in a sea of opposite spins. For *any* initial state, a sufficiently large system will have many such metastable defects and the system will necessarily freeze. The number of these metastable scales exponentially with the total number of spins N. In contrast, on even-coordinated lattices the number of metastable defects states grows as a slower, stretched exponential function of N and they affect the asymptotic relaxation in more subtle ways.

We study the homogeneous Ising model with Hamiltonian $\mathcal{H}=-J\Sigma_{\langle ij\rangle}\sigma_i\sigma_j$, where $\sigma_i=\pm 1$ and the sum is over all nearest-neighbor pairs of sites $\langle ij\rangle$. We assume initially uncorrelated spins with $\sigma_j(t=0)=\pm 1$ equiprobably, which evolve by zero-temperature Glauber dynamics [1], corresponding to a quench from $T=\infty$ to $T=0$. We focus on d-dimensional hypercubic lattices with linear size L and periodic boundary conditions. Most of our results continue to hold for free boundary conditions and on arbitrary even-coordinated lattices.

Glauber dynamics at zero temperature involves picking a spin at random and computing the energy change ΔE if the spin were flipped. For $\Delta E<0$, $=0$, or >0, the flip is accepted with probability 1, 1/2, or 0, respectively. After each event, the time is updated by $1/L^d$ so that each spin undergoes, on average, one update attempt in a single time unit. In practice, we update only flippable spins (those with $\Delta E\leqslant 0$) and update time by 1/(number of flippable spins) after each spin flip event. For each initial state, one realization of the dynamics is run until the final state. At $T=0$, metastable states in this dynamics have an infinite lifetime that can prevent the equilibrium ground state from being reached. This is the basic reason why dynamics at $T=0$ is different from that of small positive temperature.

To understand the long-time behavior in general dimensions, it is helpful to consider initially the soluble case of one dimension [5]. For $T=0$ Glauber kinetics, the expectation value of the ith spin, $s_i\equiv\langle\sigma_i\rangle$, obeys the diffusion equation and therefore the average magnetization $\langle m\rangle=(1/L)\Sigma_j s_j$ is conserved [1]. Since there are no metastable states in one dimension, the only possible final states are all spins up or all spins down. For initial magnetization $m(0)$, a final magnetization $m(\infty)=m(0)$ can be achieved only if a fraction $\frac{1}{2}[1+m(0)]$ of all realizations of the dynamics ends with all spins up and a fraction $\frac{1}{2}[1-m(0)]$ with all spins down.

On the square lattice, there exist a huge number of metastable states that consists of alternating vertical (or horizontal) stripes whose widths are all $\geqslant 2$. These arise because in zero-temperature Glauber dynamics, a straight boundary between up and down phases is stable; a reversal of any spin along the boundary increases its length and raises the energy. However, a stripe of width 1 is unstable because it can be cut in two at no energy cost by flipping one of the spins in the stripe.

The mere existence of these metastable states implies that a finite sample may not reach the ground state. However, one could expect that the probability to reach such stripe states approaches zero as the system size grows; $\lim_{L\rightarrow\infty}P_{\rm str}(L)$

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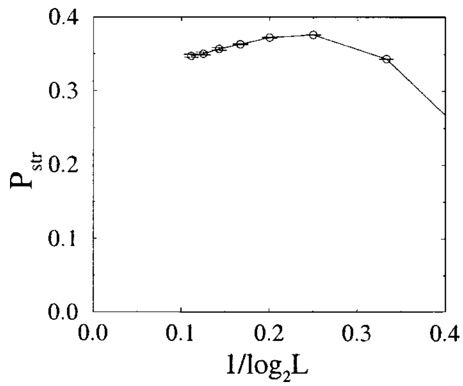

FIG. 1. Probability that an $L\times L$-square eventually reaches a stripe state, $P_{\rm str}(L)$, as a function of $1/\log_2 L$ for $L\le 512$. Each data point (with error bars) is based on 10^6 initial spin configurations for $L\le 64$ and 10^5 configurations for $L\ge 128$.

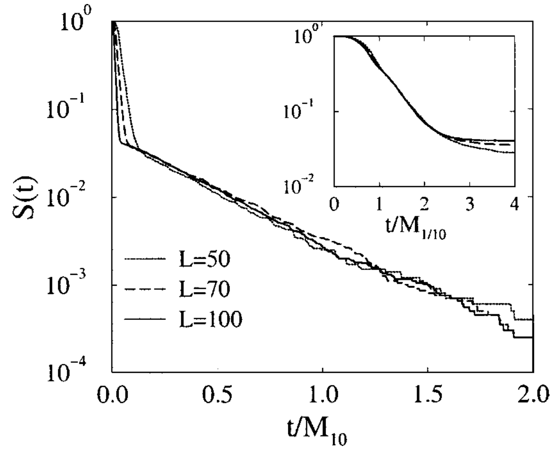

FIG. 3. Time dependence of the survival probability $S(t)$ on $L\times L$ squares. Main graph: $S(t)$ versus t/M_{10} to highlight the long-time exponential tail. Here $M_k\equiv\langle t^k\rangle^{1/k}$ is the kth reduced moment of the time to reach the final state. Scaling sets in after $S(t)$ has decayed to approximately 0.04. Inset: $S(t)$ versus $t/M_{1/10}$ to highlight the scaling and the faster exponential decay in the intermediate-time regime.

$=0$. Our simulations on $L\times L$-squares with $L\le 512$ appear to disagree with this expectation (Fig. 1), where extrapolation of $P_{\rm str}(L)$ as $L\to\infty$ suggests a nonzero value close to 0.3. Numerically, we also find that states with more than two stripes almost never appear.

When the two-stripe state is reached on the square lattice, both stripes have width typically of the order of $L/2$. There is also a gradual narrowing of the continuous component $C_{2d}(m)$ of the final magnetization distribution, $F_{2d}(m)=\frac{1}{2}(1-P_{\rm str})[\delta(m-1)+\delta(m+1)]+P_{\rm str}C_{2d}(m)$, which appears to converge to a finite-width limit as $L\to\infty$ [Fig. 2(a)]. On the simple cubic lattice, there are many more metastable state topologies and also relatively more states with narrow stripes so that there is a larger probability that the final magnetization is close to ± 1. The final magnetization distribution also exhibits good data collapse even at relatively small system sizes. Strikingly, the final magnetization distribution on the cubic lattice is well fit by $F_{3d}(m)=\frac{3}{4}(1-m^2)$ [Fig. 2(b)].

Intriguing behavior is also exhibited by the survival probability $S(t)$ that the system has not yet reached its final state by time t. On the square lattice, $S(t)$ is controlled by two different time scales. On a semilogarithmic plot, $S(t)$ lies on a straight line with a large negative slope and then crosses over to another line with smaller negative slope at long times (Fig. 3). In the intermediate time regime, the energy decays as $t^{-1/2}$ as expected [2]. The crossover in $S(t)$ occurs when domains, which grow according to the classical $t^{1/2}$ law [2], reach the system size leading to the crossover time $\tau_c\propto L^2$.

Quite surprisingly, the source of the long-time anomaly in $S(t)$ arises from the approximately 4% of the configurations in which a diagonal stripe appears (Fig. 4). On the torus, this configuration consists of one stripe of ↑ spins and another of ↓ spins which, by symmetry, have width of order $L/2$. Each

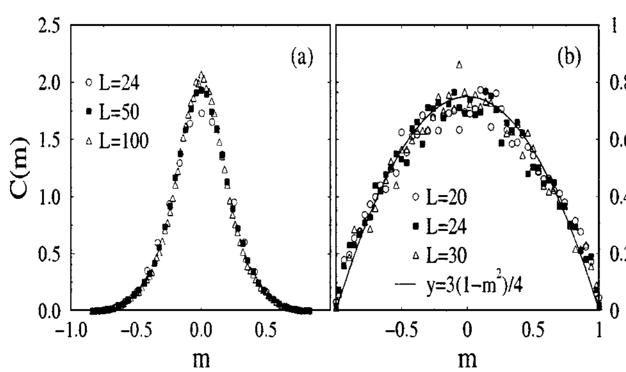

FIG. 2. Final magnetization distribution on the (a) square and (b) cubic lattices. On the square lattice, this distribution narrows as L increases but appears to reach a nonsingular limit. On the cubic lattice, data collapse occur even at small sizes. The number of realizations is 10^5 for the square and $\ge 10^4$ for the cubic lattices.

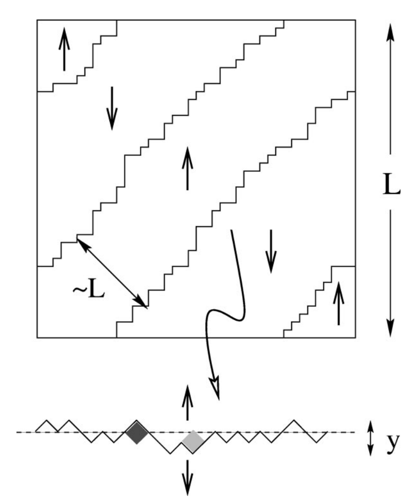

FIG. 4. Diagonal stripe configuration on the square lattice with periodic boundaries. The lower portion shows part of one interface rotated by 45°. Zero-temperature Glauber dynamics is equivalent to particle deposition at the bottom of a valley (light-shaded square) corresponding to the spin-flip event ↑→↓, or particle evaporation from a peak (filled square), corresponding to ↓→↑.

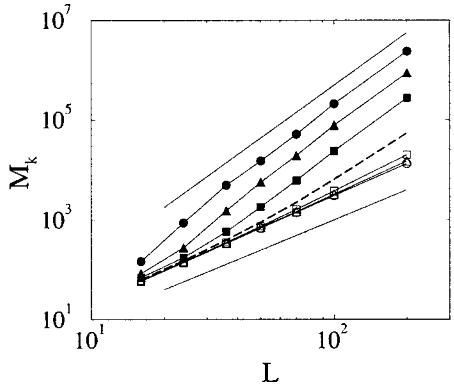

FIG. 5. Dependence of $M_k \equiv \langle t^k \rangle^{1/k}$ on L. Shown are the cases $k=1$ (dashed curve), $k=1/2$ (□), 1/4 (△), and 1/10 (○) as well as $k=2$, 4, and 10 (corresponding filled symbols). The thin straight lines have slopes 2 and 3.5.

of these stripes winds once both toroidally and poloidally on the torus; they cannot evolve into straight stripes by a continuous deformation of the boundaries. Consequently a diagonal stripe configuration ultimately reaches the ground state.

Diagonal stripes are also extremely long lived. For $L=200$, for example, the time for such a configuration to reach the final state is two orders of magnitude larger than the typical time which is of order L^2. To understand this long lifetime, we view a diagonal boundary as an evolving interface in a reference frame rotated by 45° [6].

In this frame (Fig. 4 lower), a spin flip is equivalent either to ''particle deposition'' at the bottom of a valley ($\uparrow \to \downarrow$) or ''evaporation'' from a peak ($\downarrow \to \uparrow$). In a single time step each such event occurs with probability 1/2. For an interface with transverse dimension of order L, let us assume that there are of the order of L^μ such height extrema. Reference [6] predicts $\mu=1$, but we temporarily keep the value arbitrary for clarity. Accordingly, in a single time step, where all interface update attempts occur once on average, the interface center-of-mass moves a distance $\Delta y \sim L^{\mu/2}/L$ to give an interface diffusivity $D \sim (\Delta y)^2 \sim L^{\mu-2}$. We then estimate the lifetime $\tau_{\rm diag}$ of a diagonal stripe as the time for the interface to move a distance of order L to meet another interface. This gives $\tau_{\rm diag} \sim L^2/D \sim L^{4-\mu}$. Using the results of Ref. [6], we expect $\tau_{\rm diag} \propto L^3$.

The survival probability reflects these two time scales (Fig. 3) and their L dependence is clearly visible in the reduced moments $M_k \equiv \langle t^k \rangle^{1/k}$ of the time until the final state is reached. The main contribution to the moments with $k<1$ comes from short-lived configurations, while for $k>1$ the main contribution comes from long-lived diagonal-stripe configurations. Our data for M_k with $k<1$ scales approximately as L^2, while for $k>1$, M_k scales roughly as $L^{3.5}$, somewhat faster growth than expected from the interface analogy (Fig. 5).

In greater than two dimensions, the probability to reach the ground state rapidly vanishes as the system size increases. For example, $P_{\rm gs}=1-P_{\rm str} \approx 0.04$ and 0.003 for cubic lattices of linear dimension $L=10$ and 20. For larger lattices, the ground state has not been reached in any of our simulations. One obvious reason why the system ''misses'' the ground state is the rapid increase in the number of metastable states with spatial dimension. This proliferation of metastable states makes it more likely that a typical configuration will eventually reach one of these states rather than the ground state. Another striking feature is that many metastable states in three dimensions form connected iso-energy sets, while metastable states are all isolated in two dimensions. Thus a three-dimensional system can end up wandering forever on one of these connected sets.

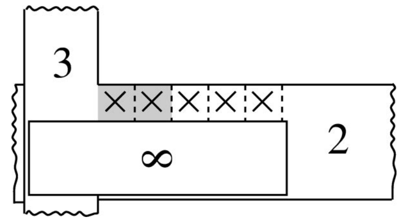

FIG. 6. A stochastic blinker on the cubic lattice. The sites marked by the × can ''blink'' between height 3 (shaded) and 2 with a step in between.

A specific example from a simulation on a small cube is sketched in Fig. 6. By viewing the spins as cubic blocks, the cluster of aligned spins appears as a ''building'' with a two-story section (marked 2), an adjacent three-story section (marked 3), and a section (marked ∞) that wraps around the torus in the vertical direction and rejoins the building on the ground floor. The wiggly lines indicate that building sections also wrap around in the x and y directions.

The sites marked by × are ''blinkers.'' Consider the leftmost such site of height 2. Since there are three directions where the nearest neighbors are part of the building, this leftmost spin can flip with zero energy cost. If this occurs, then its right neighbor, which was initially stable, can now flip with no energy cost. This motion can continue up to the right edge of the ∞ section of the building but no further. Therefore the interface between height 2 and height 3 performs a random walk, constrained to move forever in the interval marked by the × sites. This construction arises naturally on even-coordinated Cayley trees and thus appears to be generic in high dimensions.

Another feature of the final state is that it almost always consists of only two interpenetrating clusters that both percolate in all three Cartesian directions. These two percolating clusters must each contain no convex corners to be stable at $T=0$. While there are also metastable states with many components and those with components percolating in one or in two directions, such configurations are generally not reached when the system is large enough.

The energy decay on the cubic lattice also suggests that there exist more than one relaxational time scale. Initially, the energy decreases systematically in a manner consistent with a power-law decay. At longer times, however, the energy exhibits plateaux of increasing duration punctuated by small energy decreases. Ultimately the final energy is reached after which constant-energy stochastic blinking occurs *ad infinitum*. Our data for the time until the appearance of the first energy plateau scales roughly as L^3, while the time to reach the final energy seems to increase faster than any power of L.

The phase-space structure of the metastable states appears to be a crucial element in understanding the fate of Ising ferromagnets. The simplest aspect is to estimate the number of metastable states $M_d(N)$ as a function of the spatial dimension d and number of spins $N=L^d$. In two dimensions, a metastable state contains alternating horizontal or vertical stripes of up and down spins with each stripe of width $\geqslant 2$. This is identical to the number of ground states of a periodic Ising chain with nearest-neighbor ferromagnetic interaction J_1 and second-neighbor antiferromagnetic interaction J_2 [axial next-nearest neighbor Ising (ANNNI) model], when $J_2=-J_1/2$. For the chain with open boundaries, the number of metastable state was previously found in terms of the Fibonacci numbers [7]. For the periodic system the number of metastable states is

$$M_2=\frac{g^{L-1}-(-g)^{-L+1}}{\sqrt{5}}-\frac{2}{\sqrt{3}}\sin\frac{\pi}{3}(L-1)+2, \qquad (1)$$

where $g=\frac{1}{2}(1+\sqrt{5})$ is the golden ratio and the first term is just the ANNNI model degeneracy. Equation (1) therefore gives $M_2(V)\sim e^{A_2\sqrt{N}}$ with $A_2=\ln g$.

For $d=3$, we may give a lower bound for the number of metastable states by generalizing the stripe states of the square lattice. Consider states that consist of an array of straight filaments such that each filament cross-section is rectangular and the ''Manhattan'' distance between any two rectangles is $\geqslant 2$. The number of packings of such filaments is of the order of $\exp(cL^2)$, where c is a constant. This gives the lower bound for the number of metastable states, $M_3(N)>\exp(cN^{2/3})$. This same construction in d dimensions gives $M_d(N)>\exp(cN^{(d-1)/d})$. While we have not succeeded in constructing an upper bound, it seems plausible that this bound has the same form as the lower bound and hence $M_d(N)\sim\exp(A_dN^{(d-1)/d})$. In addition, we have verified that the number of metastable states on the Cayley tree grows exponentially with the number of spins [8]. Thus metastable states become relatively more numerous as the dimension increases and their influence on long-time kinetics should correspondingly increase.

In summary, the homogeneous Ising ferromagnet exhibits surprisingly rich behavior following a quench from infinite to zero temperature. On the square lattice, there appears to be a nonzero probability of reaching a static two-stripe state. Evolution via a diagonal stripe configuration is responsible for a two-time-scale relaxation kinetics. On the cubic lattice, the probability of reaching both the ground state or a frozen metastable state vanishes rapidly as the system size increases. The system instead reaches a finite iso-energy attractor of metastable states upon which it wanders stochastically forever.

Note added. After this paper was completed, we learned of related work on anomalies in the kinetics of the $T=0$ Ising-Glauber system [9]. We thank A. Lipowski for informing us of this work.

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