

Prediction of logarithmic growth in a quenched Ising model

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We study the growth of domains following a quench in an Ising model with weak next-nearest-neighbor antiferromagnetic bonds. These bonds introduce energy barriers to coarsening of the domains and thus lead to slow dynamics. In three dimensions, simple physical arguments suggest that the barriers are proportional to the characteristic length scale L for quenches below T_E , the edge-roughening transition temperature. This should lead to logarithmic growth of L at long times. Monte Carlo simulations are not totally conclusive, but do provide support for logarithmic growth.

When a system is quenched from high temperatures to a temperature below the order-disorder transition, domains form and coarsen. Of particular interest is how the characteristic coarsening length scale $L(t)$ grows with time t .¹ Originally there were theoretical predictions that some simple-model systems, in particular the Ising model with spin-exchange dynamics (which conserves the order parameter)² and the Potts model with $q \geq d+1$,³ would show logarithmic growth of domains at long times. For a while, such claims could not be disproved since the numerical evidence was ambiguous due to long-time transients and finite-size effects. However, large Monte Carlo and Monte Carlo renormalization-group studies, bolstered by theoretical arguments, have shown that, in fact, the long-time growth in these models obeys the laws $L(t) \sim t^{1/3}$ or $t^{1/2}$, respectively.⁴ Indeed, the only models known to exhibit logarithmic domain growth are those which contain randomness explicitly in their Hamiltonians, such as the random-field Ising model and spin glasses.¹ In light of these results and on the basis of appeals to the concept of universality, there seems to be a growing belief that dimensionality and details of the Hamiltonian do not matter, so that all nonrandom systems with dynamics that do not conserve the order parameter will exhibit $t^{1/2}$ domain growth at long times.⁵

Motivated by the slow dynamics present in glasses,⁶ we have been looking for a counter example—a model without randomness which nonetheless has energy barriers to coarsening that grow with L . Such growing barriers would readily lead to logarithmic growth,¹ as will be shown below. We believe we have found these growing barriers in one of the simplest frustrated models one can imagine, namely a three-dimensional Ising model with weak antiferromagnetic next-nearest-neighbor (NNN) bonds.

Consider an Ising model on a hypercubic lattice in d dimensions with ferromagnetic nearest-neighbor (NN) bonds and antiferromagnetic NNN bonds. The Hamiltonian for this system is

$$H = -J_1 \sum_{\text{NN}} s_i s_j + J_2 \sum_{\text{NNN}} s_i s_j, \quad (1)$$

where the s_i take on the values -1 and $+1$. With this sign convention, both J_1 and J_2 are positive quantities. We require $J_1/J_2 > 2(d-1)$, so that the ground state for

this model is ferromagnetic.⁷ The dynamics are chosen as single-spin flip, and thus the order parameter is not conserved.

The following simple physical argument demonstrates that the NNN bonds introduce barriers to domain coarsening. Consider shrinking a droplet of, say, up spins immersed in a sea of down spins.⁸ We can imagine that this is a necessary process in the coarsening.⁹ First, we consider a square droplet in a two-dimensional system. Without the NNN bonds, such a square can shrink away without the system having to cross any energy barriers, since a corner flips without energy cost, and then the edges can also unravel without energy cost. However, the NNN bonds introduce an energy barrier of $4J_2$ to flipping a corner spin, since three of its four NNN spins are pointing down. Once the corner flips, then the edges can flip without energy cost. Therefore, shrinking the square involves surmounting several barriers of height $E = 4J_2$. Note that the barriers to be crossed are independent of the edge length L . For time scales smaller than a characteristic time $\tau = \exp(4J_2/T)$, little domain coarsening occurs. However, on time scales much longer than τ , such corner flips occur regularly and a $t^{1/2}$ law is observed.¹⁰ In the language of Lai, Mazenko, and Valls,¹ this is a class-2 system.

In three dimensions, the argument for flipping a cube of linear size L , shown in the inset in Fig. 1, is made in an analogous fashion. The energy barrier to flip a corner is now $12J_2$. The new twist that enters is that there is now a barrier of $4J_2$ to flip each edge spin. Since to flip an entire edge requires that the corner spin flip and then each edge spin flip in turn, the barriers add and the total barrier to remove an entire edge is $E = 4(L+1)J_2$. (Once an entire edge has flipped, there are other smaller energy barriers involved in further shrinking the cube. However, in the low- T or high- L limit, the largest of the barriers that must be crossed in series dominates the time of flip the cube.) The time to flip a cube is $t \sim \tau_0 \exp[4(L+1)J_2/T]$. Inverting this equation for the edge length L of the smallest cubes which will remain at a time t , we find

$$L(t) \sim \frac{T}{4J_2} \log(t/\tau_0) - 1, \quad (2)$$

giving us the commonly known result¹ that energy bar-

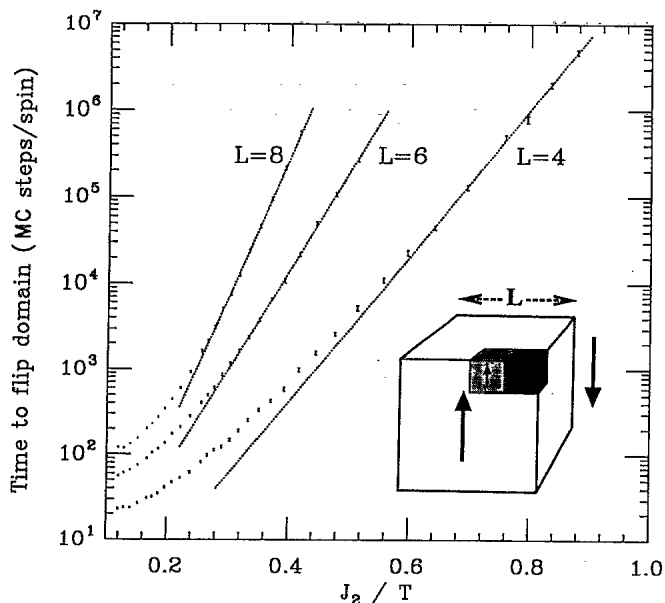


FIG. 1. Shrinking a cube of up spins embedded in a sea of down spins. Each point represents Monte Carlo results averaged over 144 runs. The lines are linear least-squares fits through the lower-temperature points, and their slopes on this Arrhenius plot give the energy barrier E . As expected, the energy barrier to shrinking cubes grows with L . The energy barriers obtained from the fits, 19.6 ± 0.5 , 26.5 ± 0.3 , and 37.0 ± 0.3 (in units of J_2) for $L=4$, 6, and 8, respectively, are in reasonably good agreement with the prediction $E(L) = 4J_2(L+1)$ (Ref. 15). (These runs are with $J_1/J_2 = 6$. Runs for larger values of J_1/J_2 yield nearly identical results.) The inset shows how this prediction was obtained. A corner spin (dark gray) has nine of its twelve next-nearest neighbor NNN spins pointing down (as can be seen by counting the number of visible edges of the corner cube), and thus there is an energy barrier of $12J_2$ to flipping it. After a corner flips, each spin along the edge (light gray) can flip in turn, but there is an energy barrier of $4J_2$ for each flip, because seven of the twelve NNN spins are pointing down. The total energy barrier is thus $E(L) = 12J_2 + 4J_2(L-2) = 4J_2(L+1)$.

riers which diverge with the characteristic size $L(t)$ of the coarsening domains should lead to logarithmically slow growth in $L(t)$.

We can imagine two possible objections to this argument. The first is that we are interested not in energy barriers but in *free-energy* barriers. The effects of entropy must be accounted for. In particular, our argument in three dimensions relies on the assumption that thermal fluctuations do not introduce a large population of free steps on faces. That is, we assume that faces are smooth and edges are sharp. It is, in fact, well known that faces will remain smooth below the roughening temperature T_R ($\approx 2.4J_1$ for $J_2=0$).¹¹ When $J_2 > 0$, there is also a finite transition temperature T_E below which edges remain sharp.¹² We can obtain an estimate of T_E for an infinite edge by studying a one-dimensional model of a step unbinding from an edge.¹³ Solving this model numerically using transfer-matrix methods,¹⁰ we find that T_E varies from $\sim 1.6J_1$ for $J_1/J_2=6$ to $\sim 0.59J_1$ for $J_1/J_2=200$. [A simple mean-field-type argument gives T_E implicitly

via the formula $J_2 e^{2J_1/T_E} = 2T_E$ and demonstrates that T_E is of order J_1 , up to factors like $\log(J_1/J_2)$.] However, the finite length of the edge of a cube means that an edge can roughen from the corners inward, without there having to be a jag in the edge which costs J_1 energy. An approximate calculation of the free-energy barrier accounting for this effect suggests an edge-roughening temperature $T_E \approx 9J_2$.¹⁰ We expect that the edge roughens and our argument breaks down near the lower of these two estimates for T_E . For temperatures below T_E , our argument should be valid.

The second objection to our argument is that although we have found energy barriers which scale with L , we have not proven that the system cannot somehow get around these barriers, i.e., that it can coarsen without having to cross them. To construct such a proof would be very difficult since it requires a detailed understanding of the spin configurations which form in a quench. The next best way to attempt to answer this objection is by doing numerical simulations. We have simulated the system using Monte Carlo (MC) techniques, with random updating of the spins. Since the runs are done at low temperatures where most spins will not flip in one time step, we employ the continuous time algorithm of Bortz, Kalos, and Lebowitz¹⁴ to greatly increase the speed of our program.

In order to confirm the most basic claim in our argument, we first investigate shrinking cubic domains of up spins in a sea of down spins. The results of these simulations are shown in Fig. 1. At low temperatures, in which the time for shrinking of the domain is dominated by the largest of the series of barriers that must be crossed, the data fall approximately on a straight line on this Arrhenius plot. The energy barrier (given by the slope of this line) increases with the size of the cube, and is in good agreement¹⁵ with the expected value of $4J_2(L+1)$.¹⁶

Next, we consider quenching a three-dimensional system from $T_{\text{init}} = \infty$ (a random spin configuration) to some final temperature T . The growth of $L(t)$ is shown in Fig. 2.¹⁷ After a short period of faster relaxation on very short length scales, the growth is approximately a power law $t^{n_{\text{eff}}}$ with the effective exponent n_{eff} for the domain growth (given by the slope on this log-log plot) increasing from ~ 0 for large values of J_2/T to $\sim \frac{1}{2}$ for $J_2/T=0$. Such power-law growth with temperature-dependent effective exponents has been seen before in Monte Carlo results both in models where growth is $t^{1/2}$ and in models where it is logarithmic in t at long times.^{1,18} However, we feel that in this case the results are more compatible with logarithmic growth at long times for three reasons.

First, we can get an estimate of the largest barrier heights involved in the coarsening process out to the times studied by noting that at $t=10^5$ MC steps/spin and $J_2/T = \frac{1}{3}$, the time is almost 3 orders of magnitude larger than the time taken for equivalent coarsening in a system with $J_2=0$. Such a difference in time scales corresponds to barrier heights of about $20J_2$.¹⁹ That such large energy barriers exist in the system suggests that the process involves the cooperative flipping of many spins, lending strong support to our argument. Admittedly, however, such a barrier height is that associated with flipping an edge of length 4, while $L(t)$ is about three times this

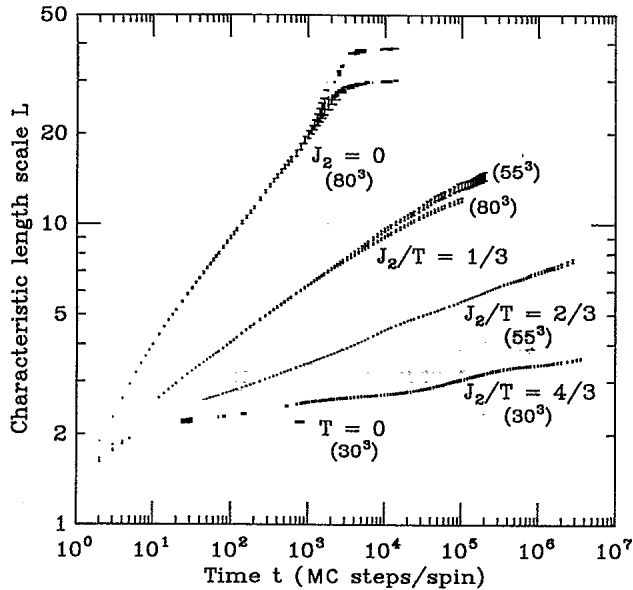


FIG. 2. Coarsening of domains following a quench from $T_{\text{init}} = \infty$. For each value of J_2/T , the values of $L(t)$ represent an average over ten Monte Carlo runs. The numbers in parentheses give system sizes. Note that the introduction of the NNN bonds leads to a dramatic slow down in the growth of the domains. Over the times studied, there appears to be no crossover toward $t^{1/2}$ behavior and, in fact, for $J_2/T = \frac{1}{3}$, the slope is decreasing at late times, lending support to the claim of logarithmically slow growth at asymptotically long times. Since this curvature for $J_2/T = \frac{1}{3}$ becomes even a bit more pronounced when system size is increased from 55^3 to 80^3 , it is unlikely to be due to finite-size effects. (These runs are for $J_1/J_2 = 6$. For $J_1/J_2 = 24$, flips which increase the J_1 contribution to the energy are essentially prohibited over the times studied but the results are very similar, with the downward curvature for $J_2/T = \frac{1}{3}$ a bit more pronounced.)

large. We believe this is due to the fact that the system is not well-characterized by simply one length. There are a distribution of lengths in the system (as is apparent when we look at the spin configurations during the coarsening) and the processes which occur will be those associated with the shortest length, since these will be the fastest. However, the entire distribution of lengths should diverge as the system coarsens and thus the growth should still be logarithmic in t .

Second, there is no evidence that the growth is crossing over to $t^{1/2}$ [as clearly occurs in quenches of two-dimensional systems¹⁰ once the time is on the order of $\exp(4J_2/T)$] and, in fact, there is downward curvature in Fig. 2 for $J_2/T = \frac{1}{3}$. This is what we would expect for logarithmic growth. Of course, such results must be interpreted with some caution, since it is known that finite-size effects can become important when $L(t)$ is only a small fraction of the system size,²⁰ and our periodic boundary conditions would tend to produce downward curvature, as

is apparent for the runs for $J_2 = 0$. However, the curvature for $J_2/T = \frac{1}{3}$ is occurring at a shorter length scale than that at which finite-size effects produce curvature for $J_2 = 0$, and, furthermore, the curvature becomes even slightly more pronounced as we increase the system size from 55^3 to 80^3 . Therefore, we believe that the downward curvature is a real effect.

Third, we have observed the spin configurations which occur during the quench. In contrast to spin configurations for the unfrustrated ($J_2 = 0$) model, the configurations at long times in this model are clearly blocklike, with a preference for large flat faces aligned along the simple cubic directions.¹⁰ Thus the system seems to be getting stuck in just the sort of configurations we expect it should.

In conclusion, we have considered the growth of domains following a quench in an Ising model with weak antiferromagnetic next-nearest-neighbor bonds. For the three-dimensional case, a simple physical argument suggests, but does not conclusively prove, that the asymptotic domain growth in this model is logarithmic in time when the system is quenched below a temperature T_E , the roughening temperature for domain edges. The argument rests on an estimate of the time needed to shrink a cubic domain immersed in a larger domain of oppositely oriented spins. Numerical simulations confirm the correctness of this estimate for small cubes. They show further that for quenches of an initially random spin configuration, there are indeed large barriers which produce slow coarsening. At the longest times studied, these barriers are large enough that they are almost certainly due to processes involving the collective flipping of at least a few spins. There is no evidence of a crossover to $t^{1/2}$ behavior and, in fact, there is some evidence of a crossover to logarithmic growth at long times. We believe that the logarithmic coarsening of domains may, in fact, be quite common in three-dimensional frustrated systems.

Note added in proof

The effect exponent n_{eff} for the MC runs with $J_2 = 0$ (and $T = \frac{1}{8} J_1$) in Fig. 2 is actually about 0.35 rather than $\frac{1}{2}$. Similar deviation from the expected $L(t) \sim t^{1/2}$ behavior has previously been observed for the three-dimensional Ising model at zero temperature by Amar and Family.²¹

Shah and Mouritsen²² have reported some numerical evidence for logarithmic coarsening in another model without randomness, namely the two-dimensional Ising model with annealed vacancies.

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- ⁴For the Ising model with conserved order parameter see, e.g., D. A. Huse, *Phys. Rev. B* **34**, 7845 (1986); J. G. Amar, F. E. Sullivan, and R. D. Mountain, *ibid.* **37**, 196 (1988); C. Roland and M. Grant, *ibid.* **39**, 11971 (1989). For the Potts models see, e.g., J. Viñals and M. Grant, *Phys. Rev. B* **36**, 7036 (1987); G. S. Grest, M. P. Anderson, and D. J. Srolovitz, *ibid.* **38**, 4752 (1988). Most of the work has concentrated on two-dimensional systems. We do not, in fact, find the evidence against logarithmic growth in three-dimensions to be completely convincing.
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- ⁶For discussion of slow dynamics in glasses see J. P. Sethna, J. D. Shore, and M. Huang (unpublished).
- ⁷For equilibrium properties of the two-dimensional model, see J. Oitmaa, *J. Phys. A* **14**, 1159 (1981).
- ⁸An argument based upon the shrinking of such droplets was used by G. Grinstein and J. F. Fernandez [*Phys. Rev. B* **29**, 6389 (1984)] to demonstrate the logarithmic growth of domains in the random field Ising model.
- ⁹Actually, this statement may not be true for the three-dimensional model, since in the initial random configuration, the density of both up and down sites ($p=0.5$) is well above the percolation threshold ($p_c \approx 0.312$). [D. Stauffer, *Introduction to Percolation Theory* (Taylor and Francis, London, 1985)]. This means most sites are part of the two infinite clusters. Finite clusters, particularly of large size, are quite rare. (This has been confirmed by both combinatorics and numerical study.) We do not believe this to be a problem because our argument should still hold for "handles" on the infinite clusters.
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- ¹³Since such a model neglects roughening fluctuations on the faces, the value obtained is an upper bound on the true T_E .
- ¹⁴A. B. Bortz, M. H. Kalos, and J. L. Lebowitz, *J. Comp. Phys.* **17**, 10 (1975).
- ¹⁵In fact, our simulation results are still not in the low-temperature limit ($T/J_2 \approx 2$ or 3), and the extent of agreement of the slope E_s on the Arrhenius plot with our predicted zero-temperature barrier $E_0 = 4J_2(L+1)$ is somewhat fortuitous. If we look instead just at the time to depin the first step from an edge, we find values of E_s which increase more rapidly with L , e.g., $E_s = 41.3 \pm 0.6$ (as compared to the predicted value $E_0 = 36$) for $L=8$. This slope is due partly to the free-energy barrier itself and partly to the decrease of this barrier with increasing temperature. [We can study this analytically by doing an approximate expansion of the partition function in powers of $\exp(-4J_2/T)$. The predicted values thus obtained, e.g., $E_s = 41.9$ for $L=8$, are then in much better agreement with the simulation results (see Ref. 10).] Shrinking the whole cube gives a lower slope because it involves surmounting several more barriers of smaller size.
- ¹⁶What if the domain is not initially a cube? We also investigated shrinking spherical domains of radius R , and confirmed that the domain still gets stuck in configurations with flat faces. The average time to shrink the domain is in rough agreement with the expectation that the barrier is determined by the largest cube contained inside the sphere, namely one with edge length $L = R/\sqrt{3}$.
- ¹⁷We have measured the characteristic length scale as the inverse perimeter of the domain boundaries: $L(t) = -E_0^n / (E^n - E_0^n)$, where E^n is the energy associated with nearest-neighbor bonds only and $E_0^n \equiv -3NJ_1$ is this energy in the ground state. For discussions on the various possible definitions of $L(t)$, see D. Chowdhury, M. Grant, and J. D. Gunton, *Phys. Rev. B* **35**, 6792 (1987).
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- ¹⁹Since the behavior is not very sensitive to the ratio J_1/J_2 , activation over J_2 —and not J_1 —barriers is what is important here. Our simulations do not go out far enough in time to rule out the possibility that at long times the system can avoid the growing J_2 barriers by going over large, but L -independent, J_1 barriers, although such a scenario seems unlikely.
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- ²¹J. G. Amar and F. Family, *Bull. Am. Phys. Soc.* **34**, 491 (1989); and (private communication).
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