LOGARITHMICALLY SLOW COARSENING IN NONRANDOMLY FRUSTRATED MODELS

Joel D. Shore, James P. Sethna, Mark Holzer, and Veit Elser
Physics Department, Cornell University, Ithaca, New York 14853

ABSTRACT

We study the growth ("coarsening") of domains following a quench in an Ising model with weak next–nearest–neighbor antiferromagnetic (AFM) bonds and single–spin–flip dynamics. The AFM bonds introduce free energy barriers to coarsening and thus greatly slow the dynamics. In three dimensions, simple physical arguments suggest that the barriers are proportional to the characteristic length scale $L(t)$ for quenches below the corner rounding transition temperature T_{CR}. This should lead to $L(t) \sim \log(t)$ at long times t. Monte Carlo simulations provide strong support for this claim.

We also predict logarithmic growth in a purely two–dimensional tiling model, which can be thought of as describing a single interface in our three–dimensional model viewed from the [111] direction. Here, the slow coarsening dynamics should persist all the way up to the order–disorder transition (at T_{CR}). However, if the model is cooled slowly at a rate Γ, the final length scale should have power–law, not logarithmic, dependence on $1/\Gamma$. Simulations support both of these claims.

INTRODUCTION

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 length scale $L(t)$ grows with time t at long times.

Historically, there have been some theoretical predictions that certain systems without randomness in their Hamiltonians would show logarithmically slow coarsening at long times.[1] 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 simulations, bolstered by more careful theoretical arguments, eventually showed that the long time growth in these models obeys the naively–expected power laws: $L(t) \sim t^n$ with $n = 1/3$ or $1/2$ (depending on whether the dynamics does or does not conserve the order parameter, respectively).[2] 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.

In light of these results, there seems to be a growing belief that, for nonrandom systems quenched to nonzero temperature, the $n = 1/3$ and $n = 1/2$ power law behavior is universal (*i.e.*, independent of the details of the Hamiltonian), and even independent of the dimensionality. Motivated by the slow dynamics present in glasses,[3] we have been looking for counter examples, *i.e.*, models without randomness which display logarithmically slow ordering dynamics.[4]

ARGUMENT FOR LOGARITHMICALLY SLOW GROWTH

Consider the nearest–neighbor Ising ferromagnet on a square or cubic lattice in $d = 2$ or 3 dimensions, with frustration added by introducing weak next–nearest–neighbor (NNN) antiferromagnetic (AFM) bonds. The Hamiltonian is

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

where $s_i = \pm 1$. The first sum is over all nearest–neighbor (NN) bonds while the second is over all NNN bonds. We have chosen our sign convention so that both J_1 and J_2 are positive when

the NN bonds are ferromagnetic and the NNN bonds are antiferromagnetic. We will require that $J_1/J_2 > 2(d-1)$ so that the ground state for this model is ferromagnetic. We will study this Hamiltonian under single–spin–flip (*i.e.*, nonconserved) dynamics.

The NNN AFM bonds introduce free energy barriers to coarsening and thus greatly slow the dynamics (freezing the system completely at $T = 0$). In two dimensions, these barriers are independent of the characteristic length scale $L(t)$, and thus $L(t) \sim t^{1/2}$ at long times.[4] Let us now study what happens in three dimensions by considering the time to shrink a cubic domain of, say, up spins in a larger sea of down spins (see inset of Fig. 1). The energy barrier to flip a corner spin (black cube) is $12J_2$. Once a corner flips, the neighboring spins along an edge (white cube) can flip in turn, but there is an energy barrier of $4J_2$ for each to flip. The barrier to flip the spins along an entire edge is then $E = 4J_2(L+1)$, where L is the linear size of the domain. The time t to do this is given by activation over this barrier and is thus exponential in L:

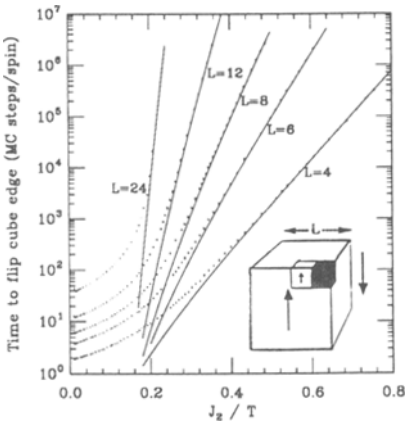

Fig 1. Arrhenius plot of the time to flip all the spins along the edge of a cubic domain of size L (shown in inset). Curves are the theoretical forms derived from a low temperature expansion, as discussed in the text.

$$t = \tau_0 \, e^{4(L+1)J_2/T} \, . \tag{2}$$

Naively inverting this equation to solve for the size of the smallest structure which we expect to remain in a coarsening system at time t, we find

$$L(t) \sim \frac{T}{4J_2} \log(t/\tau_0) \, . \tag{3}$$

This gives the expected result[5] that energy barriers which diverge with the characteristic length scale $L(t)$ should lead to logarithmically slow coarsening.

Of course, the above discussion is only valid in the limit $T \to 0$. What happens at nonzero temperatures where we must consider not energy barriers but, rather, *free* energy barriers? Fig. 1 shows Monte Carlo simulation results for the average time t to flip all the spins along the edge of a cubic domain. We see that the slope on this Arrhenius plot increases with domain size L, thus confirming our prediction of an activation barrier which grows with L.

Furthermore, if we write

$$t = \tau_0(T) e^{F_B(L,T)/T} \, , \tag{4}$$

we can perform a low temperature expansion for both $\tau_0(T)$ and $F_B(L,T)$.[4] The curves in Fig. 1 show the resulting prediction, which has no free parameters and is in excellent agreement with the simulation results at low temperatures.

We expect our argument for logarithmically slow coarsening to break down when the free energy barrier per unit length (to flip the spins along a cube edge) goes to zero. This occurs at the corner rounding temperature T_{CR}, which has previously been studied in the context of equilibrium crystal shapes.[6] In the limit $J_1/J_2 \to \infty$, T_{CR} can be calculated exactly[7,4] and yields $T_{CR} \approx 7.11 J_2$.

SIMULATIONS OF THE COARSENING PROCESS

There is still a large gap in our argument: Although we have identified a special configuration in which there are energy barriers that scale with the length scale L, we have not shown

that during the process of coarsening the system will necessarily find itself in configurations in which it will have to cross these barriers in order to coarsen further. It is conceivable that the system could find a path through configuration space which goes around these barriers. To construct a proof that the barriers must be crossed is very difficult since it requires a detailed understanding of the spin configurations which form in a quench. Instead, we turn to numerical simulations of the coarsening process in order to test our conjecture.

Fig. 2 shows the growth of $L(t)$ following a quench from infinite temperature (a random spin configuration) to a final temperature T. Since this is a log–log plot, power law behavior would give a straight line. We see that as the ratio of T/J_2 is decreased, the coarsening slows dramatically. Furthermore, at temperatures below T_{CR} (for $T/J_2 = 2$, 3, and 4), the Monte Carlo data show some downward curvature on this log–log plot at late times. [By contrast, for $J_2 = 0$ and $T/J_2 = 8$, there is no downward curvature until finite–size effects lead to a sharp leveling off of $L(t)$ once it is approximately 1/3 the system size.] This suggests that the growth is becoming slower than a power law. In fact, if we replot this on a log–normal plot we find that, while there is considerable upward curvature at early times, the last one to two decades of data are quite straight and thus in reasonably good agreement with logarithmic growth of $L(t)$.[4]

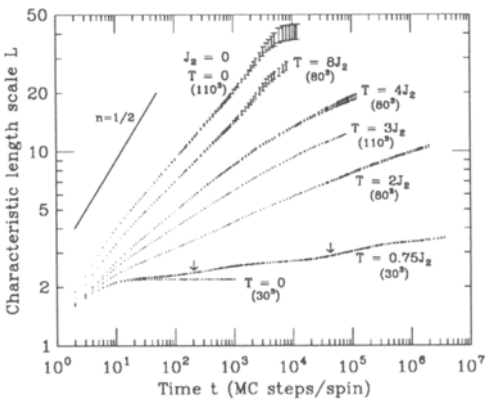

Fig 2. Growth of $L(t)$ following a quench from infinite temperature to a final temperature T. Numbers in parentheses give system sizes.

THE TILING MODEL

We now briefly discuss a closely related model which is also expected to show logarithmic coarsening. This is a two–dimensional model for a single interface in the three–dimensional model as viewed from the [111] direction. If we require that the configurations of this interface have no bubbles or overhangs (when viewed from this direction), then we obtain the so–called "[111]–restricted solid–on–solid (RSOS) model" for our three–dimensional model.[7] The RSOS restriction corresponds to taking the limit $J_1/J_2 \to \infty$ in the 3-d model. Any configuration in the RSOS model (of which an example is shown in Fig. 3) can be represented as a tiling of the plane by 60° rhombi of three different orientations. (The model also has a third representation as an Ising spin system on a triangular lattice.[7])

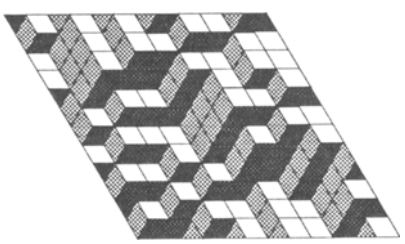

Fig 3. A sample configuration for the tiling model.

The order–disorder transition in this model occurs at T_{CR}. Above T_{CR}, the interface is rough (*i.e.*, the tiles intermingle); below T_{CR}, the interface forms a sharp corner (*i.e.*, the tiles phase separate). When the system is quenched from infinite temperature to $T \leq T_{CR}$, we expect that the interface will coarsen under the dynamics, which consists of adding or removing cubes subject to the RSOS restriction. Since this dynamics conserves the order parameter in

this model, the naively–expected behavior would be $L(t) \sim t^{1/3}$. However, the mechanism by which the interface coarsens involves activation over precisely the same sort of barriers which grow with $L(t)$ as in the three–dimensional model. Thus, the same arguments we made for logarithmically slow coarsening in the three–dimensional model should apply here as well. Simulations of the coarsening process once again lend support to this claim.

Unlike in the three–dimensional model, here the ordering temperature and the temperature at which the dynamics becomes slow coincide. Thus, we might hope that this system would be glassy, *i.e.,* that it would have great difficultly ordering even when cooled slowly at a rate Γ. Specifically, we'd want the final ($T = 0$) value of L to depend only logarithmically on the time $1/\Gamma$ spent cooling. We have simulated slow cooling in this model and find that this does not appear to be the case. Furthermore, more careful arguments suggest that we should expect $L(T = 0) \sim \Gamma^{-1/4}$ in the limit $\Gamma \to 0$, which is in reasonably good agreement with the simulation results.[4] The reason why the dependence is a power law and not a logarithm is because the free energy barrier goes continuously to zero at T_{CR}, and thus there is a region of temperature just below T_{CR} where the barriers are small and the system can still coarsen quite rapidly.

CONCLUSIONS

We have discussed two closely related models in which we conjecture that the growth of the domains should be only logarithmic in time following a quench. Simulations lend strong support to this conjecture. However, if cooled slowly at a rate Γ, these models are not expected to order sluggishly: the final domain size has a power law, rather than a logarithmic, dependence on $1/\Gamma$.

ACKNOWLEDGEMENTS

We thank David Huse, Peter Nightingale, Jennifer Hodgdon, and David DiVincenzo for helpful discussions. This work was supported in part by NSF Grant No. DMR 88-15685 and computing facilities were provided in part by the Cornell–IBM Joint Study on Computing for Scientific Research.

REFERENCES

1. S. A. Safran, Phys. Rev. Lett. **46**, 1581 (1981); G. F. Mazenko, O. T. Valls, and F. C. Zhang, Phys. Rev. B **31**, 4453 (1985).
2. D. A. Huse, Phys. Rev. B **34**, 7845 (1986); J. Viñals and M. Grant, Phys. Rev. B **36**, 7036 (1987); G. S. Grest, M. P. Anderson, and D. J. Srolovitz, Phys. Rev. B **38**, 4752 (1988); J. G. Amar, F. E. Sullivan, and R. D. Mountain, Phys. Rev. B **37**, 196 (1988); C. Roland and M. Grant, Phys. Rev. B **39**, 11971 (1989).
3. For more details, see J. P. Sethna, J. D. Shore, and M. Huang, to appear in Phys. Rev. B (Sept. 1991); and references therein.
4. More details on the work presented here can be found in J. D. Shore, Ph.D. thesis, Cornell University (1992). An earlier report on some of the work is given in J. D. Shore and J. P. Sethna, Phys. Rev. B **43**, 3782 (1991).
5. Z. W. Lai, G. F. Mazenko, and O. T. Valls, Phys. Rev. B **37**, 9481 (1988).
6. C. Rottman and M. Wortis, Phys. Rev. B **29**, 328 (1984).
7. A.-C. Shi and M. Wortis, Phys. Rev. B **37**, 7793 (1988); and references therein.