Transient and Asymptotic Domain Growth in the 3D Ising model with Conserved Spin

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Abstract

We present a study of domain growth in the three-dimensional Ising model with locally conserved magnetization. For the first time in a dynamical Ising model, the theoretically expected growth exponent $n = 1/3$ is confirmed; we observe it over a wide range of temperatures. For low temperatures, the transient phenomena are accurately described by a mean-field model. The algorithm used for this study allows different types of transport processes to be controlled, and can be applied to many other problems.

After a binary mixture is quenched across a demixing phase transition, it does not separate into its coexisting phases instantaneously. Instead, domains of the coexisting phases grow, their size often increasing as a power law of time. This phenomenon has been studied extensively for binary alloys [1], liquid mixtures [2] and polymer blends [3]. The simplest models for this coarsening process are dynamical Ising models with locally conserved magnetization. The coarse-grained magnetization of these models is believed to be described by a Langevin equation (so-called Model B) [4]. If one phase occupies a small volume fraction, the theory of Lifshitz, Slyozov and Wagner (LSW) [5] suggests that the domain size R will grow as a power-law in time, $R \approx t^n$, with $n = 1/3$. The same exponent has been observed in simulations of Model B in two and three dimensions [6], and in the two-dimensional Ising model with locally conserved magnetization [7] over a large range of volume fractions. However, this exponent has never been observed in a three-dimensional dynamical Ising model, and arguments exist for other growth laws in this model [8].

This paper firmly establishes the existence of power-law domain growth with an exponent of $n = 1/3$ in a dynamical Ising model with spin-exchange dynamics. This power-law behavior occurs after a long transient regime, the length of which we have been able to measure for the first time. We do this by introducing a new algorithm for conserved-spin dynamics which is of general applicability to lattice models. In the problem discussed in this paper we obtain an increase in computational efficiency of about 10^{115} at $T = 0.01T_c$ over the Kawasaki spin exchange dynamics [9] that are usually used in such studies. Finally, for low temperatures the transient phenomena are accurately described by a simple mean-field model.

The Hamiltonian of the Ising model is:

$$H/k_BT = -J \sum_{<i,j>} \sigma_i \sigma_j \tag{1}$$

where a spin σ_i is located at position r_i and can take the values ± 1, and where $< i, j >$ denotes a pair of neighboring sites. For conserved total spin, the Hamiltonian can be rewritten:

$$H/k_BT = -4J \sum_{<i,j>} \delta(\sigma_i, 1)\delta(\sigma_j, 1) \tag{2}$$

up to an additive constant, where $\delta(\alpha, \beta)$ is the Kronecker delta function. In our algorithm,

for each site, we keep track of its coordination number (number of neighbors with equal spin value): $Q(j) = \sum_{<i,j>} \delta(\sigma_i, \sigma_j)$. All sites j for which $Q(j) = q$ are stored in a list with N_q elements.

One step of our algorithm for a three-dimensional cubic lattice consists of:

a) increment time [10] by $\Delta t = 1/\sum_q [(1 - q/6)N_q \exp(-4Jq)]$.

b) select list q with probability $P_q = \Delta t(1 - q/6)N_q \exp(-4Jq)$

c) select randomly one site i from list q.

d) select randomly a neighbor j of site i, with $\sigma_j \neq \sigma_i$.

e) flip σ_i and σ_j, adjust the Q-values of i, j and their neighbors, and update the lists.

The transition rate from configuration A to configuration B for this algorithm is given by:

$$T_{A\to B} = \frac{1}{\Delta t} P_q \frac{1}{N_q} \frac{1}{6-q} = \frac{1}{6} \exp(-4Jq) \tag{3}$$

in which the factors arise from steps a, b, c, and d respectively. ¿From this equation, detailed balance [11] can be easily verified, which in addition to ergodicity guarantees that equilibrium is described by the Boltzmann distribution for Hamiltonian (1).

One can obtain Kawasaki dynamics by selecting a pair of neighboring sites $< i, j >$ with probability proportional to $\exp[-2J(Q(i) + Q(j))]$ instead of selecting a site i with probability proportional to $\exp[-4JQ(i)]$, and randomly one of its neighbors j. This small change has dramatic consequences for the dynamical behavior. Compare a 'free' spin (with $q = 0$) to a 'bound' spin adjacent to a flat interface (with $q = 1$). For our new dynamics, the rate for a move of the bound spin along the interface is $\exp(-4J)$ times smaller than the rate for the free spin diffusing in the bulk; in Kawasaki dynamics, both spins move with equal rates. Thus, surface diffusion is suppressed in our algorithm, relative to Kawasaki dynamics. This suppression increases tremendously at low temperatures. Note that the transition rates for all moves in the bulk diffusion of an isolated spin (i.e. detachment, bulk transport and

reattachment) in our dynamics are identical to those in Kawasaki dynamics. Therefore the time-scales of the two algorithms may be directly compared. In the LSW theory, the late-time growth is due to the dominance of bulk diffusion over all other transport processes. Suppression of surface diffusion should reduce the domain size at which bulk diffusion starts to dominate, thus enabling us to reach the scaling region both earlier and with smaller lattices.

To study domain growth, we quenched the three-dimensional Ising model on a 64^3 simple-cubic lattice from infinite temperature (where $J = 0$ and the spins are randomly ± 1), to below the critical temperature (J larger than the critical coupling $J_c = 0.22163$). After the quench, we let the system evolve using the dynamics described above. To measure the typical domain size R, we calculate the two-point correlation function $g(|r|, t) = \sum_i \sigma(r_i)\sigma(r + r_i)$ and determine its first zero-crossing: $g(R, t) = 0$ [12]. In Figure 1 we have plotted $R(t)$ for final temperatures $T/T_c = 0.7$, 0.5, 0.4, 0.3, 0.2, 0.15 and 0.01, for which equilibrium interface widths (thermal correlation lengths) are less than one lattice spacing [13]. In each case, there is a transient regime in which $R(t) \leq 2$, followed by an asymptotic regime where $R(t)$ shows an approach to power-law growth. The duration of the transient regime increases drastically as $T \to 0$.

At low temperature, steps in $R(t)$ can clearly be seen. These steps are rounded at higher temperatures. They correspond to a series of decays of fundamental excitations: the sites with zero coordination number (isolated spins) wander until they find a more stable environment, followed by the sites with coordination number one (spins adjacent to smooth domain walls and pairs of spins), and so on [14].

These steps may be further understood by considering the evolution of the coordination number distribution N_q. Figure 2(a) shows N_q over the course of a simulation, after a quench to $T = 0.05T_c$. The transient behavior of the N_q may be divided into 'decays', during which one of the N_q falls off over about one decade in time, and 'plateaus', during which all of the N_q are essentially constant. One can clearly see the sharp (exponential) decays of N_0, N_1, N_2 at successively later times. After each decay, the time step in our simulation grows by about a factor of $\exp(4J)$: this enables us to reach extremely large times for low temperatures.

At lower temperatures, the plateaus stretch while the decays continue to require about one decade.

The initial dynamics of N_q are well described by a simple mean-field theory. In a cubic lattice with N sites, the initial values for N_q immediately after a quench from $T = \infty$ are given by $N_q(0) = 2^{-6} N \left(\begin{smallmatrix} 6 \\ q \end{smallmatrix} \right)$ in the limit of large N. Suppose we exchange spins at neighboring sites i and j. If $Q(i) = a$ and $Q(j) = b$ before the move, then after the move, N_a and N_b are decreased by one, and N_{5-a} and N_{5-b} are increased by one.

Next we consider a neighbor of site i. If it has the same spin as site i before the flip, the probability that this spin has coordination number q is $qN_q/(\sum_k kN_k)$. After the flip, N_q is reduced by one. There are a such spins neighboring i and b such spins neighboring j. If, on the other hand, the neighbor had spin different from $\sigma(i)$, the probability that it has q identical neighbors is $(6-q)N_q/(\sum_k (6-k)N_k)$. There are $10-a-b$ such spins next to site i and j together. Finally, the probability to select two sites i and j with a and b identical neighbors is proportional to $P_{a,b} = \exp[-4Ja](6-a)N_a(6-b)N_b$. The increase in time is $(\Delta t)^{-1} = \sum_{k=0}^{6}(1-k/6)N_k \exp(-4Jk)$

Putting everything together leads to the following set of rate equations for the N_q:

$$\begin{aligned} \frac{dN_q}{dt} \;=\; & (\Delta t)^{-1} \sum_{a=0}^{5}\sum_{b=0}^{5} \left(P_{a,b} / \sum_k \sum_l P_{k,l} \right) \Bigg((10-a-b) \frac{(6-(q-1))N_{q-1}}{\sum_k (6-k)N_k} \\ & + (a+b) \frac{(q+1)N_{q+1}}{\sum_k kN_k} - (10-a-b) \frac{(6-q)N_q}{\sum_k (6-k)N_k} \\ & - (a+b) \frac{qN_q}{\sum_k kN_k} + \delta_{q,5-a} + \delta_{q,5-b} - \delta_{q,a} - \delta_{q,b} \Bigg) \end{aligned} \tag{4}$$

Figure 2(b) shows the solution of these equations for $T = 0.05T_c$. The agreement with the simulation (Figure 2(a)) is good, up to the point where N_2 begins to decay. Agreement up to longer times can presumably be achieved by keeping track of the correlations between second-nearest and more distant neighbors. In both Figure 2(a) and Figure 2(b), the time step increases by a factor of $\exp(4J)$ after each rapid decay; this is evident from the dependence of the time step on the N_q. The transient regime of the simulation ends and the asymptotic regime begins when N_3 starts to decay, at a time proportional to $\exp(12J)$.

Why does the scaling regime begin when N_3 begins to decay? What makes N_3 different from N_0, N_1 and N_2? Apparently, configurations without 'corner' sites (with $q = 3$), such as bicontinuous networks without 'dangling ends' are not attractors of our dynamics. The class of scaling states that our dynamics tends to occupy consists of domain patterns with at least dangling ends, if not isolated domains. Our rate equations for nearest neighbor coordinations select a scaling state in which in addition, N_2 has not decayed exponentially, but the general behavior is similar to that of the simulation.

To extract the power-law exponent for late times $n_{\rm eff} = \lim_{t \to \infty} (d \log R / d \log t)$ from our simulation results, we generated a set of 16 $R(t)$ curves for each anneal temperature. We then constructed 50 samples from each set using the bootstrap technique [15]. For each sample we carried out a least-square fit of the $(\log(t), \log(R))$ data to the form $\log(R) = n_{\rm eff} \log(t/t_0) + \exp(-c \log(t/t_1))$, in the regime where $R \geq 2.0$. The second term in this function corrects for the transient behavior just before the asymptotic regime. Our results are $n_{\rm eff} = 0.37(3)$, $0.35(2)$, $0.31(4)$, $0.28(2)$, $0.30(3)$, $0.33(3)$ and $0.32(3)$, for $T/T_c = 0.01$, 0.15, 0.2, 0.3, 0.4, 0.5 and 0.7, respectively. This is the first demonstration of domain growth in a dynamical Ising model in three dimensions with an exponent close to $n = 1/3$. This exponent has been observed in simulations of domain growth in Model B [4] at critical concentration. Our results suggest that our dynamics are in the Model B growth kinetics universality class.

If we rescale the time for each simulation by the characteristic time $\tau = \exp(12J)$, the asymptotic $R(t)$ curves collapse. This is illustrated in Figure 1 by the dashed lines $R(t) = A[t/\tau]^{1/3}$, with $\tau = \exp(12J)$ and $A = 1.6$, which fall close to the asymptotic $R(t)$ values from the simulations, over a large range of temperatures and times. Thus, the typical time scale in the asymptotic regime is set by the binding energy for a spin with three aligned neighbors.

In Figure 2(a), N_q for $q = 3, 4, 5$ appear to approach power-law decays with exponents close to -1/3. This can be easily understood from the scaling hypothesis, which predicts a single scale R for the domains and thus that domain walls occupy a fraction $1/R$ of the system volume [4]. For R much bigger than the domain wall thickness (thermal correlation

length), the fractions of the domain wall regions made up of $q = 3, 4$ and 5 sites should be independent of R. Thus they should each decay as $t^{-1/3}$. Obviously this requires N_6 to approach its equilibrium value with the same power law.

In summary, we have observed domain growth according to LSW theory for the first time in a dynamical 3D Ising model. This has been done by the use of a new dynamics, which, compared to Kawasaki dynamics, has identical bulk diffusion but suppresses surface diffusion. At low temperatures, the transport is highly activated, leading to a postponement of the scaling regime to a time of order $\tau = \exp(12J)$. This strong activation explains why $n = 1/3$ was not previously observed in the 3D Ising model, particularly at low temperatures. We have also presented a novel mean-field approximation for the dynamical behavior. In its crudest form, it quantitatively describes the early stages of our simulations, during which the number of sites with coordination number zero and one decay successively.

Our method for simulating 3D Ising kinetics will be useful in the study of a variety of problems. We have developed a related model which stimulates surface diffusion and suppresses bulk diffusion, along with including next-nearest neighbor interactions, which is tailored to the study of equilibrium crystal shapes. Our methods could also be effective in studying non-equilibrium crystal shapes or other interfacial kinetics. It is straightforward to account for surface fields in order to model non-equilibrium wetting kinetics, spinodal decomposition near surfaces, and lattice-gas kinetics in porous media. Ising models have well-known equilibrium phase diagrams and are preferable to Langevin equations for these types of studies.

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FIG. 1: Solid curves indicate simulation results for the domain size R as a function of time t, after a quench from $T = \infty$ to (from left to right) T/T_c =0.7, 0.5, 0.4, 0.3, 0.2, 0.15 and 0.01. The asymptotic behavior is well described by the dashed lines, which are the power laws $R(t) = A[t/\tau]^{1/3}$, with $\tau = \exp(12J)$ and $A = 1.6$. Note that the (logarithmic) time scale is contracted in the range 10^{12} to 10^{112} in order to show the lowest temperature data.

FIG. 2: Number of sites N_q with coordination number q, as a function of time after a quench from $T = \infty$ to $T = 0.05T_c$. Results are obtained from (a) simulation on a 64^3 cubic lattice, and (b) our mean-field model.