Structure and evolution of quenched Ising clusters

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The properties of domains generated following a quench from very high temperatures ($T \gg T_c$) to low temperatures are studied for an Ising model evolving under conserved or nonconserved dynamics. Before the quench the clusters satisfy percolation statistics, since T is too large for the interactions to be relevant. However, after the quench to low temperatures, we observe that the largest clusters are still percolationlike for large distances in that they are described by the same Hausdorff dimension as percolation clusters. For short distances the clusters are compact. At intermediate distances, the large clusters appear to be more fractal than percolation clusters. We interpret this intermediate regime as a crossover between a constant density at short distances and percolationlike low-density regime for large distances, not as a new type of fractal.

I. INTRODUCTION

The kinetics of an Ising system which has been rapidly quenched from a high temperature, far above the critical temperature T_c to a final temperature less than T_c has been well studied.[1] We know that the time evolution of the system depends in a crucial manner on whether the spin direction is conserved and satisfies Kawasaki dynamics or is nonconserved and satisfies Glauber dynamics. In the latter case,[2–8] the correlation length R grows algebraically as $t^{1/2}$ in both two and three dimensions, where t is the time. This result has been well documented by both analytical[2–6] and computer simulation studies,[4,7,8] as well as by experimental studies[3] on ordering alloys (e.g., Fe-Al and Cu-Au). The corresponding result for the conserved case[9–20] is less clear. It is widely believed that for the very late stages, the growth of clusters is by evaporation and condensation and, as first suggested by Lifshitz and Slyozov,[9] the average domain radius R grows as $R \cong t^{1/3}$, again for both two and three dimensions. However, this regime is difficult to reach and most Monte Carlo simulations[15–20] as well as experimental measurements[21–26] usually do not reach this late stage of growth. Instead, growth is dominated by coalescence and dissociation of small clusters which move with an effective diffusion constant. In this regime, it is often observed that $R \cong t^n$, where n is in the range 0.1—0.2. Simulations[15–20] suggest that $n \cong 0.2$ for quenches near the critical concentration (equal concentration of up and down spins), though there are suggestions that $n \cong 0.3$ when the concentration of the minority spins is small,[20] and the Lifshitz-Slyozov[9] mechanism should be more applicable. There is a suggestion[14] that at the critical concentration, $R \simeq \ln t$ for long times, as the symmetry between the up and down spins is never broken and there is no reason that Lifshitz-Slyozov type behavior should occur. Our results for the conserved system support this idea.

In addition to studies of the domain-growth kinetics, it has been shown that for both the conserved and nonconserved Ising models, the structure function, $S(k,t)$, which is the angular averaged Fourier transform of the nonequilibrium spatial correlation function, satisfies dynamic scaling[1] of the form

$$S(k,t)=\kappa^{-d}(t)F(k/\kappa(t)), \quad t>t_0 . \tag{1}$$

Here $\vec{k}$ is the wave vector measured relative to the Bragg positions of the ordered structure, $\kappa(t)$ is a characteristic time-dependent wave number, d is the dimensionality, and t_0 is an initial transient time. $F(x)$ is a scaling function which is different for conserved and nonconserved models. Scaling has been observed in both Monte Carlo simulations[1,7,15–20] and experimentally.[1,21–26] It also can be shown to be valid analytically.[1,6] While this formulation of the problem describes many of the macroscopic features of domain growth, it would be of interest to study in more detail the properties of these two systems in real space. By so doing, we hope to be able to understand the growth mechanisms more completely, particularly for the conserved model, where the long-time Lifshitz-Slyozov[9] regime is so elusive.

Our earlier work on the Q-component nonconserved Potts model[27] suggested that the topology and domain shapes evolved continuously with Q. As Q decreases, we observed that the grains become less compact. In the limit that Q is 2, the domains are no longer topologically connected and the Potts model reverts to the Ising model. In the present paper we examine the shape properties of the clusters in the Ising model as a prototypical case of the very weak topology limit. In such studies it is necessary to examine very large lattices in order to avoid boundary effects at very early times. For this reason, we have carried out studies for a 1000×1000 system for the nonconserved Ising model. We were also interested in the cluster properties for the conserved model. In this case, the growth is much slower and we are able to use a smaller lattice, 400×400. In this paper we report several interesting features of the cluster evolution which we observed for these two systems.

II. PROCEDURE AND RESULTS

The model we studied is the ordinary Ising model, described by the Hamiltonian:

$$H=-J\sum_{\rm NN} S_iS_j \tag{2}$$

where $S_i=\pm 1$. The sum is over all nearest-neighbor pairs and the exchange constant $J>0$. Clusters are groups of neighboring up or down spins. If we consider up spins as occupied sites and down spins as empty sites, then we have a lattice gas model of a fluid. In all simulations we start from a high-temperature state with equal fraction of up and down spins and rapidly quench to $T<T_c$. For the nonconserved Ising model, we performed the simulations for both the triangular and square lattices of size 1000×1000 with periodic boundary conditions. For the conserved case, we used a 400×400 triangular lattice. Glauber spin-flip dynamics are employed in the nonconserved Ising model, in which a trial spin is chosen at random and an attempt to flip it is made. The transition probability is given by

$$W=\begin{cases}\exp(-\Delta E/k_BT), & \Delta E>0\\ 1, & \Delta E\le 0\ ,\end{cases} \tag{3}$$

where ΔE is the change in energy resulting from the spin flip and k_B is the Boltzmann constant. Kawasaki spin-exchange dynamics are employed for the conserved Ising model. In this case the transition probability is for the exchange of two neighboring, unlike spins. The transition probability is

$$W=\frac{\exp(-\Delta E/k_BT)}{1+\exp(-\Delta E/k_BT)}\ . \tag{4}$$

In either case, a transition is accepted provided that W is greater than or equal to a random number r $(0\le r\le 1)$. For $W<r$, the old spin configuration is retained. We define the unit of time as 1 Monte Carlo step (MCS) per spin which corresponds to N microtrials or spin-flip attempts for the nonconserved model or N spin-exchange attempts for the conserved model.

Our starting state for high T is that of a random distribution of up and down spins. For a given configuration of the spins, the distribution of cluster sizes is just that of site percolation.[28] Since the percolation threshold p_c equals 0.50 for the triangular lattice and 0.59 for the square lattice, the initial state is either at its percolation threshold or below it. Ising clusters in thermodynamic equilibrium have been studied extensively, particularly near the critical temperature.[29–32] Here we are interested in understanding how these initial ramified, percolation clusters evolve into ordered domains after the temperature is suddenly quenched to low T below T_c. It is known that as the transition temperature is approached from above, the percolation threshold on the square lattice decreases from 0.59 to 0.50 at T_c.[33] The percolation threshold remains unchanged for the triangular lattice. Above T_c, one can describe a new percolation problem,[32,34] known as correlated site percolation, where one studies the effect of temperature correlations on the percolation problem. This new percolation problem has the same critical exponents as ordinary percolation.

In this paper we are interested in what happens well below T_c, where the large clusters grow at the expense of the smaller ones. We observe that a length L_p exists such that for $L>L_p$, clusters have the same fractal dimension as that of percolation clusters, i.e., $D=1.90$.[28] This is true for the large finite clusters and the two spanning clusters (one of up spins and one of down spins). However, L_p increases very rapidly, and for distance smaller than L_p the clusters appear to have a lower fractal dimension,[35] not higher. As time proceeds L_p increases, thereby indicating that change from one fractal regime (percolation $D=1.90$) to another is a kinetic process. Simultaneously, a second length scale L_c is also growing. For $L<L_c$, the clusters are compact, $D=2$. Both L_p and L_c must increase with time, but for L intermediate between these two lengths, the clusters are surprisingly more ramified. We observe similar results for the conserved model, but because the clusters evolve much more slowly, L_p grows slowly.

Section II A summarizes our data for the nonconserved Ising model. Similarly, the data for the conserved Ising model are presented in Sec. II B.

A. Nonconserved Ising model

In Figs. 1 and 2 we show the evolving spin configurations for the triangular and square lattices for the nonconserved Ising model, quenched rapidly from $T=\infty$ to $T=0$. The two largest spanning clusters are shaded. As is clear from these figures, the number of clusters de-

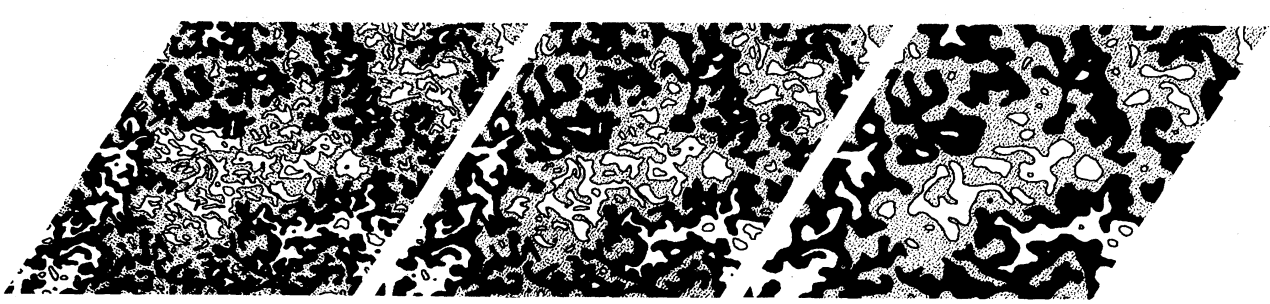


FIG. 1. Evolution of the domain boundary for the nonconserved Ising model quenched from $T\gg T_c$ to $T=0$ on a triangular lattice of size 1000×1000. The two spanning clusters are shaded.

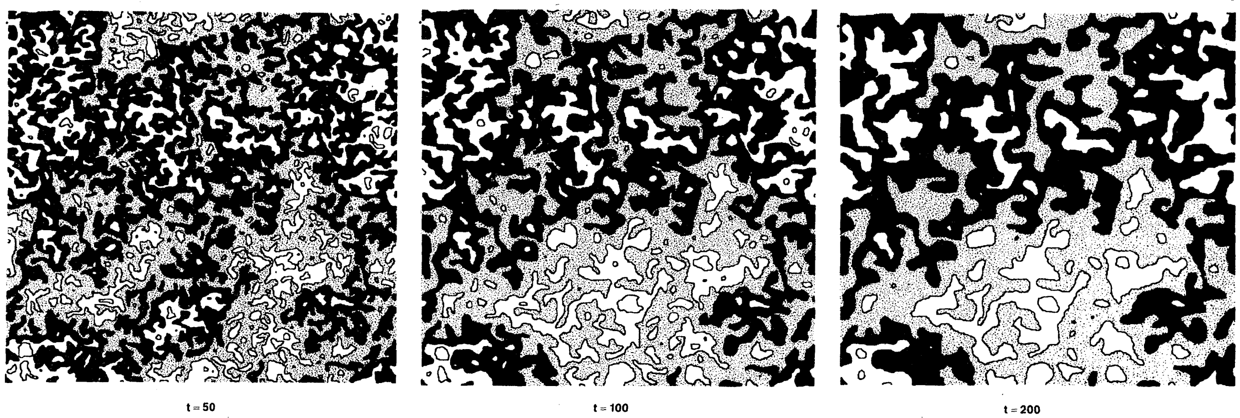


FIG. 2. Evolution of the domain boundary for the nonconserved Ising model quenched from $T \gg T_c$ to $T=0$ on a square lattice of size 1000×1000. The two spanning clusters are shaded.

creases rapidly and we do not have sufficient statistics to determine the cluster-size distribution function. After only 200 MCS/spin, there are only a few clusters remaining and approximately 80% of the spins are in one of the two large spanning clusters. As seen from the figures, the large clusters have many features of percolation clusters on long scales, but not for short and intermediate distances. In particular, there are no weak one-dimensional channels which typically connect percolation clusters. These are unstable and either become thicker or break. When they break, large pieces of the cluster are often disconnected, thereby leaving the clusters more ramified on an intermediate scale than the original percolation clusters. This picture can be justified by determining the fractal dimension of the clusters. One way to measure D is to tabulate the mass $M(r)$ of a cluster within a radius r. For a D-dimensional cluster $M(r)$ should scale[35] as r^D. In Figs. 3 and 4 we display our results as $\ln M(r)$ versus $\ln r$ for the two large spanning clusters (solid circles) as well as for large finite clusters, for the triangular and square lattices, respectively. For $t=0$, we find that $D=1.90\pm0.02$, in agreement with the known fractal dimension of a percolation cluster. However, after only 10 MCS/spin, it is clear that the region where $D=1.9$ moves out very quickly and holds only for $L > L_p$. For $L > L_p$, the eventual long-range order has not had time to propagate over distances larger than L_p and the clusters retain features of the original random-site percolation clusters. For shorter length scales, the clusters appear to be more fractal. Fitting a straight line to the region $L < L_p$, we find $D=1.74\pm0.04$ for both the triangular and square lattices. This value of D does not seem to depend on time, but we are only able to measure D between 10 and 100 MCS/spin. For longer times, the clusters are very much affected by the periodic boundary conditions, as seen from the 200-MCS configurations plotted in Figs. 1 and 2.

To check whether this lower value of D is real and not a crossover effect, we calculated the density $\rho(r)$ of sites within a given cluster. For a fractal object $\rho(r)$ should scale as r^{D-d}, where d is the dimension of space. In the present study $d=2$. Results for $\ln\rho(r)$ versus $\ln r$ are shown in Fig. 5 for three times after the system was quenched to $T=0$ on the triangular lattice. The $t=0$ results are for the largest spanning cluster and yield a Hausdorff dimension of $D=1.90\pm0.02$. For $t=50$ and 100, $\rho(r)$ has the same slope as the percolation cluster ($t=0$), confirming the discussion above. However, there is no

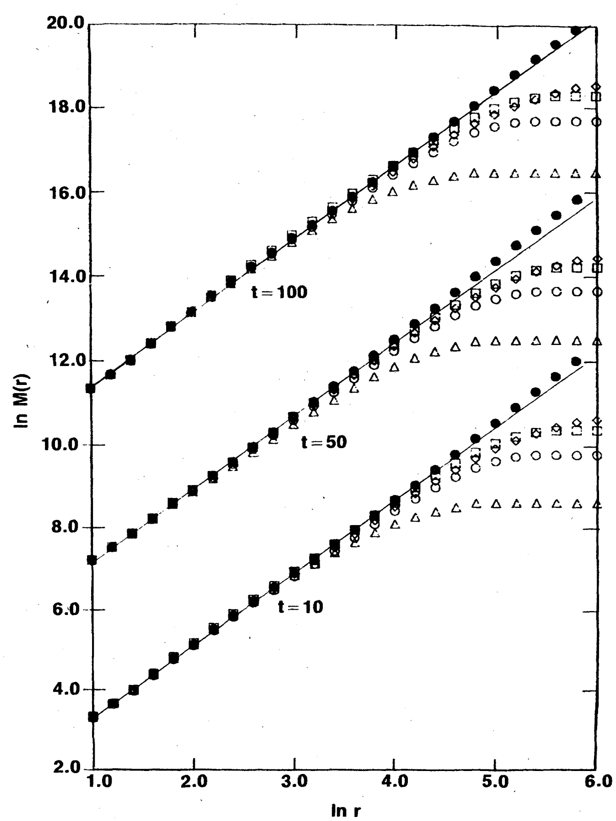


FIG. 3. $\ln M(r)$ versus $\ln r$ for one of the large spanning clusters (solid circles) and four finite clusters at three different times after the quench from $T \gg T_c$ to $T=0$ on the triangular lattice for the nonconserved Ising model. Results for $t=50$ and 100 are displaced vertically for clarity. The same finite clusters are not shown for all three times. Results for the two spanning cluster fall on top of one another.

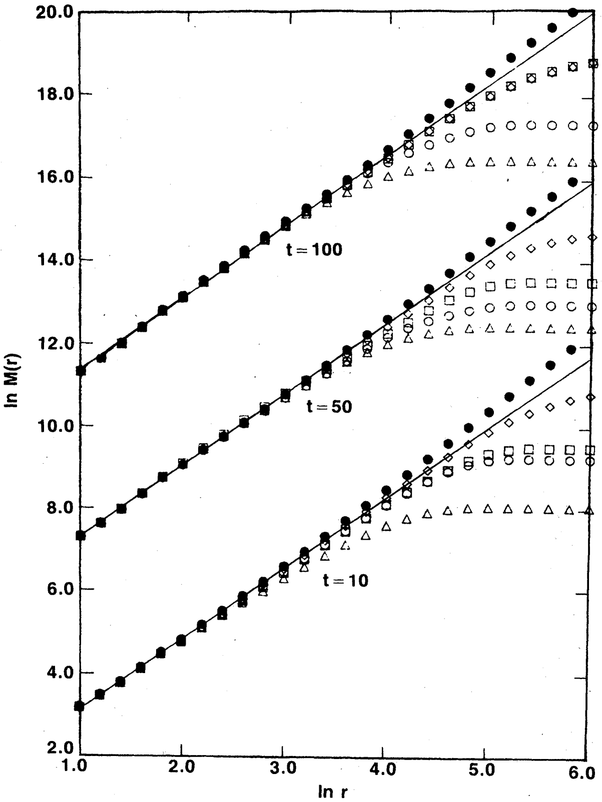


FIG. 4. $\ln M(r)$ versus $\ln r$ as in Fig. 3 for the square lattice.

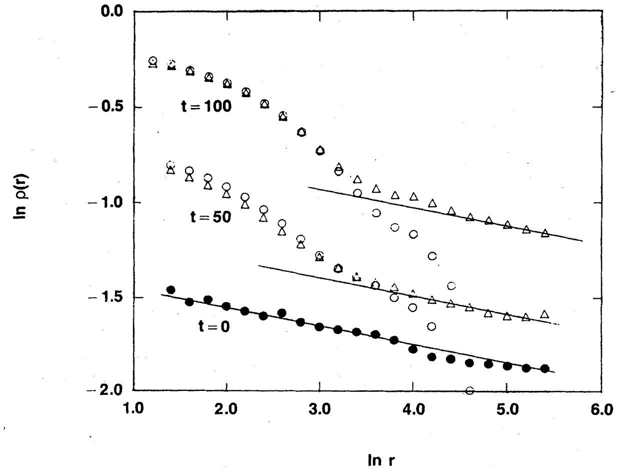


FIG. 5. $\ln\rho(r)$ versus $\ln r$ for three different times after the quench from $T \gg T_c$ to $T=0$ on the triangular lattice. The solid circles are for $t=0$, before the quench. The results for $t=100$ are displaced vertically for clarity. The open circles for $t=50$ and 100 are for one of the spanning clusters, while the triangles are for the largest nonspanning cluster. The line through the points has a slope -0.10 for all three curves, which is expected for percolation clusters (i.e., $d-D=-0.10$).

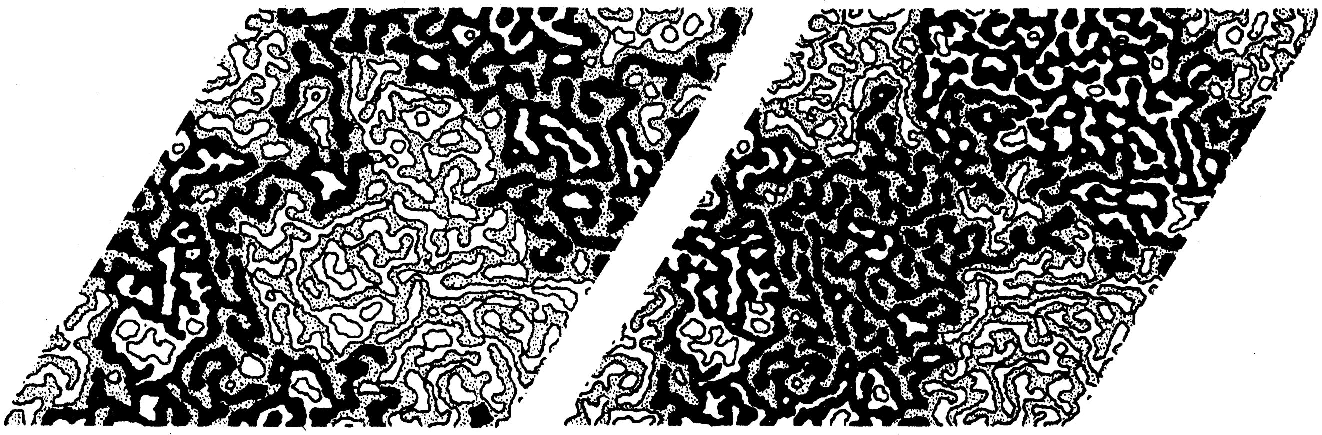
clear intermediate region, where $\ln\rho(r)$ can be fit with a straight line, indicating that the spatial region where we obtained $D=1.74$ from the mass $M(r)$ is more correctly interpreted as a crossover region. From Fig. 5 we see that for very short distances, the density $\rho(r)$ seems to be approaching a constant. This is easy to understand, since the domains are growing, and for long times the spins surrounding a given spin are very likely to be within the same cluster. For $L<L_c$, the clusters are compact and $\rho(r)$ scales as r^0 (i.e., $D=d=2$). Evidence for this lower cutoff can be seen for $t=50$ and 100 MCS in Fig. 5. However, in all of the present simulations L_c was at most a few lattice spacings.

Though it is possible to interpret the regime where $D\cong 1.74$ as a true fractal region, it is more likely a crossover effect. Since the short distance behavior has $D=2$, which means constant density, and the long-distance regime is fractal, which means $\rho(r)$ is a decreasing function of r, the only way these two regimes can be connected is by an intermediate regime which has a lower fractal dimension. What is very interesting is that the percolation properties of the clusters can still be detected at large distances. Presumably this will be true for all stages of the growth.

In addition to studying the cluster properties, we also examined the boundaries of the clusters. In particular, we measured the correlation $\rho(r)$ between lattice sites on the domain boundaries. We found that for short distances, $\rho(r)$ scaled as r^{-1}, indicating that only one boundary is being sampled and the Hausdorff dimension is $D=1$. For large distances, $\rho(r)$ scaled as r^0, suggesting compactness. The crossover between these two regimes occurred at a length scale intermediate between L_c and L_p. The observed crossover in $\rho(r)$ versus r was very sharp compared with those seen in Fig. 5. While the two values of the Hausdorff dimension observed may be simply understood, the sharpness of the transition is a surprising feature.

B. Conserved Ising model

We have carried out a similar study of the properties of the clusters for an Ising model evolving according to conserved or Kawasaki dynamics. In this case, the time scale of the growth is considerably slower than for the nonconserved case. For this reason we used a smaller system (400×400) than for the case above.[36] Figure 6 shows the evolving spin configurations on a triangular lattice for the conserved Ising model, quenched rapidly from $T=\infty$ to $T=0.6T_c$. The concentration of up and down spins were equal, $p=0.50$. The two largest spanning clusters are shaded. As is clear from Fig. 6, the system evolves much more slowly when the spins satisfy conserved dynamics rather than nonconserved dynamics. Even after 30 000 MCS/spin the clusters still have random percolation features at large distances. This is seen from a plot of the mass $M(r)$ of a single cluster within a circle of radius r (Fig. 7). For $L>L_p$, we find that $D\cong 1.90$, as expected for random percolation clusters. Note that L_p is still rather small even after 30 000 MCS/spin. If we fit a straight line to the short-distance behavior, we find $D\cong 1.66$, but as in the case of the conserved spin, we believe this is a crossover effect from a compact structure for small L and that of the more open percolation cluster for $L>L_p$. For the conserved model the short-distance



t = 16000 t = 30000

FIG. 6. Evolution of the domain boundary for the conserved Ising model quenched from $T \gg T_c$ to $T = 0.6T_c$ on a triangular lattice of size 400×400. The two spanning clusters are shaded. Note the difference in time scales between this figure and Fig. 1.

cutoff L_c is barely detectable, even from a plot of $\ln\rho(r)$ versus $\ln r$.

From the results shown in Figs. 6 and 7, we believe that one can see why it is likely that the Lifshitz-Slyozov regime is not applicable for $p = 0.5$. Below T_c, in two dimensions, both the up and down spins are at their percolation threshold, independent of the type of lattice. This means that for an infinite system one can find arbitrarily large clusters of either up or down spins. Since the Lifshitz-Slyozov regime depends on the existence of isolated domains which grow due to evaporation and condensation of single spins, it seems unlikely that this late-stage regime can ever be reached when $p = 0.5$. Mazenko, Valls, and Zhang have suggested[14] that the long-time exponent for quenches at the critical concentration should grow as $R \simeq \ln t$, instead of $t^{1/3}$ as suggested by Lifshitz and Slyozov.[9] Our simulations are not long enough to test this prediction, as we find that $n \cong 0.17$, slightly lower, but consistent with earlier Monte Carlo simulations on smaller lattices. For $p \neq 0.5$, it is likely that the late-stage exponent would be $\frac{1}{3}$, as the symmetry of the up and down spins no longer holds and the Lifshitz-Slyozov mechanism is likely to come into play. Of course for p near 0.50, the crossover to this late stage is likely to be unreachable both experimentally or in computer simulations.

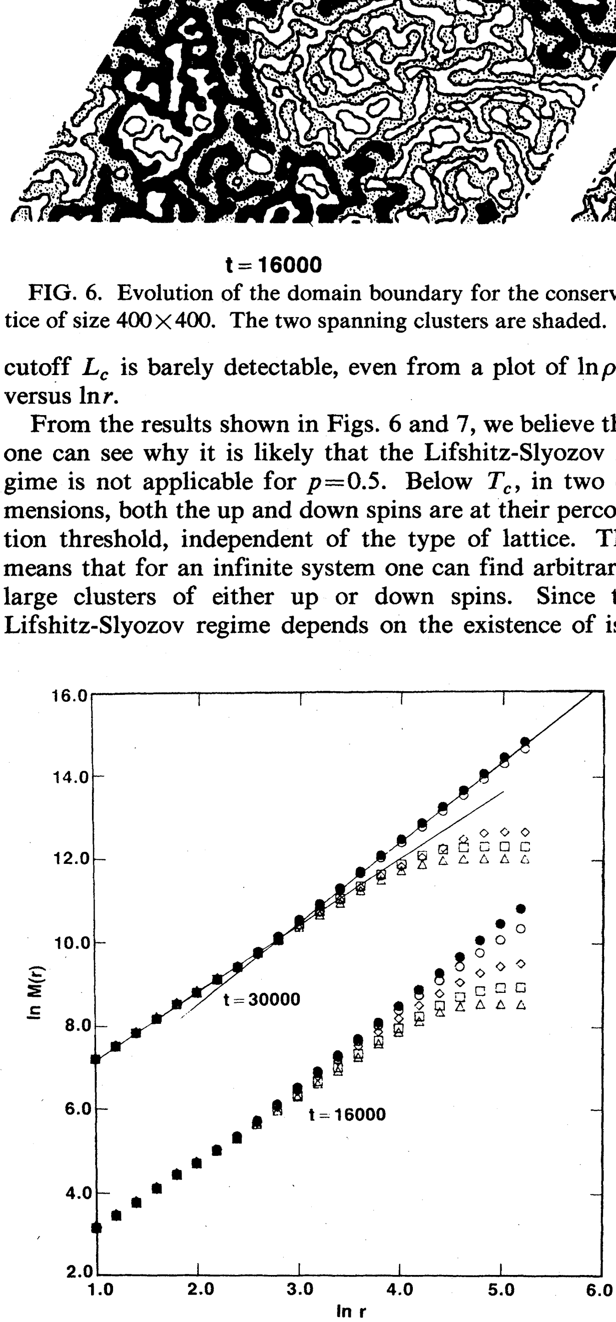


FIG. 7. $\ln M(r)$ versus $\ln r$ for the two spanning clusters (solid and open circles) and three finite clusters for the conserved Ising model after the quench $T \gg T_c$ to $T = 0.6T_c$. Results for $t = 30\,000$ are displaced vertically for clarity. The line through the data for large distances has slope equal to 1.90, while the slope of the line through data for small L has a slope of 1.66. Note that the distance L_p, where these two lines cross is rather short, even after 30 000 MCS's/spin.

III. CONCLUSIONS

We have shown how random percolation clusters evolve after a quench from high T to $T < T_c$ for the case for either conserved or nonconserved dynamics. We find that for distances larger than a characteristic length L_p, the clusters have the same fractal dimension as the original percolation clusters. As time evolves, the clusters become compact on distances shorter than L_c. At intermediate-length scales, the clusters appear to be more fractal than either the compact clusters or random percolating clusters. The decrease in the Haussdorf is attributed to the capillarity induced breaking of the weak bonds which hold the original cluster together. Though it is possible that this intermediate regime corresponds to a true fractal, we believe it is better understood as a crossover from the short distance, compact regime to the large-distance, percolation regime. For the nonconserved Ising model, this growth is extremely rapid. After only 200 MCS/spin, the effects of the finite size of our lattice (1000×1000) were becoming very important. In order to study these systems at longer times, it is necessary to employ systems with size of at least $2L_p$. However, for the case of conserved dynamics this condition is obviously satisfied since the time evolution of the system is so slow. Even after 30 000 MCS/spin, L_p was only of the order of 16 lattice spacings and our 400×400 lattice was more than adequate.

While our simulations were carried out in two dimensions, we expect similar results in three dimensions, with one difference. Since $p=0.50$ is now far above the percolation threshold, both the long- and short-distance behavior of the density is a constant, independent of r. However, since the value of this constant will be lower for $L > L_p$ than for $L < L_c$, we still expect to find an intermediate regime which appears to be more fractal.

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