Monte Carlo renormalization-group study of domain growth in the Potts model on a triangular lattice

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The kinetics of domain growth for a $q=8$ state Potts model on a triangular lattice is studied using the Monte Carlo renormalization-group technique. A block-spin transformation is applied to the evolving configurations of a two-dimensional Potts model with nonconserved order parameter. The growth law for the average size of domains is consistent with curvature-driven growth. A scaling form for the structure factor is obtained and compared to theory. The edge distribution function for the growth kinetics is also studied.

I. BACKGROUND

The kinetics of domain growth during a first-order phase transition[1] occur when a system is quenched from a high-temperature disordered phase to a temperature well below its ordering temperature T_c. In Fig. 1, we show domains of ordered phases forming and growing to macroscropic size as time goes on. This growth is often algebraic,

$$R(t) \sim t^n ,$$

where $R(t)$ is the average domain size at time t and n is the growth exponent. Experiments and computer simulations find that the spatial dependencies of such systems scale with $R(t)$. The numerical value of the growth exponent is of particular interest, because it is the signature of the thermodynamic forces driving the system to equilibrium. Growth occurs to minimize the interfacial free energy of the system. In the simplest case of a two-state nonconserved system, the Ising model, the ordering process depends on the local curvature only. This leads to an $n=\frac{1}{2}$ growth law.[2,3] Here, we study a system with many degenerate ground states ordering by nonconserved dynamics.[4-14] The system is often modeled by q-state Potts models, and experimental systems include polycrystalline materials, foams, and biological membranes.

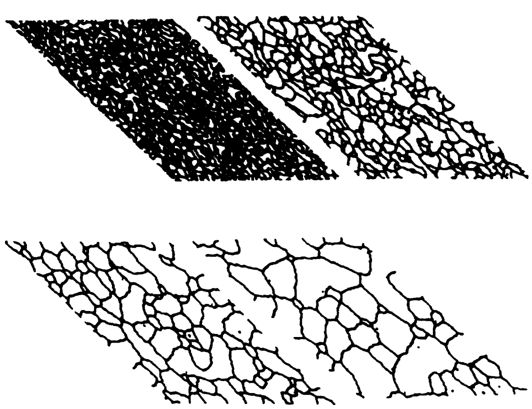

FIG. 1. Evolving domain structure of the $q=8$ Potts model on a triangular lattice of size $N=256^2$ at temperature $T=0.6$. Times shown are $t=100$, 500, 1000, and 4000 MCS, respectively.

Domain growth in nonconserved systems with many degenerate ground states has been studied by several authors. One motivation was an observation by Lifshitz,[4] which was later made more precise and useful by Safran.[5] They argued that a system with q degenerate ground states can evolve into metastable states if $q \geq (d+1)$, where d is the dimension of space. This suggested the possibility of activated growth for ordering dynamics in such systems, rather than the $q \equiv 2$ power law of $n=\frac{1}{2}$. This was investigated primarily by a convenient representation of the system: the q-state Potts model in two and three dimensions. A series of interesting papers on this and related models have been written by Grest, Srolovitz, Anderson, and co-workers;[6,7,10,11] Kaski, Nieminen, and Gunton;[8] and Kumar, Gunton, and Kaski.[9] Recently some treatments have been done which are partly motivated by the physics of foams;[12-14] the study of Nagai, Kawasaki, and Nakamura[14] provides a particularly interesting approach.

While it now seems clear that the q-state Potts model follows an $n=\frac{1}{2}$ growth law at nonzero temperatures,[8-11] initial work was hampered by the presence of strong transients. Very extensive numerical studies were required to establish the growth law, which is now thought to be independent of d and q, i.e., superuniversal. Transients lead to significant deviations in the measured growth exponent if the data analysis is performed over a limited time regime: One can obtain an effective q-dependent exponent varying from $n=0.5$ for $q=2$ to $n \approx 0.4$ for $q \geq 30$. Given these difficulties, it is of interest to find methods which avoid those transients, and permit the study of the superuniversal nature of domain growth from first principles.

In this paper, we present a Monte Carlo renormalization-group (MCRG) study of the $q=8$ state

Potts model on a triangular lattice. This addresses the nature of growth in the scaling regime from first principles. Furthermore, the scaling regime can be reached with only a modest increase in computing effort. Our results are consistent with $n=\frac{1}{2}$, and are therefore in agreement with recent studies. However, we find that MCRG gives a significant improvement in the effective exponent one measures for data taken over a limited time regime. We also present results for the structure factor and the edge number distribution functions. These are found to be invariant under the renormalization-group transformation, to the accuracy of our study.

MCRG analysis, based on a Wilson-type block-spin transformation,[15-17] has recently been applied successfully to a number of domain-growth problems: ferromagnetic kinetic Ising models with both spin-flip[18] and spin-exchange kinetics,[19] and the q-state Potts models on a square lattice.[20] The particular value of a renormalization-group study is that it is the fundamental test for the scaling properties of the system. As discussed elsewhere,[19] the renormalization-group transformation, controlled by the strong-coupling $T\rightarrow 0$ fixed point,[21] iterates away the irrelevant scaling fields of the system, allowing the direct study of asymptotic properties. Previously, Viñals and Gunton[20] studied the dynamics of the eight-state Potts model on a *square* lattice using MCRG techniques. Their results pointed to the existence of two distinct fixed points at zero temperature: a freezing fixed point associated with a logarithmic $R(t)\sim \ln t$ growth and an equilibration fixed point, which gave power-law growth. The equilibration fixed point was found to be stable at nonzero temperatures below T_c, while the freezing fixed point was only stable if the system was quenched directly to $T\equiv 0$. The existence of a freezing fixed point can be traced to frustration of the thermodynamic forces: The metastable states involve whether the lattice can be tiled with local-equilibrium shapes for domains.[20] For our purposes, since a triangular lattice cannot be tiled with hexagons of different sizes, freezing cannot occur, regardless of T. Therefore, the present MCRG study of the eight-state Potts model on a *triangular* lattice, where there are no transients due to an unstable freezing fixed point, is complementary to the work of Viñals and Gunton.

The details of our MCRG study are given below. The growth exponent we obtain, $n=0.48\pm 0.04$, is consistent with the Allen-Cahn result mentioned above, although we see evidence of a transient which gives rise to growth exponents that are considerably less than $\frac{1}{2}$. This transient is iterated away by the renormalization-group transformation, and we tentatively identify it with an effective exponent for domain growth with "soft" walls.[7,22] We also obtain the scaled structure factor and the edge distribution function.

II. METHOD AND RESULTS

A. Growth law

The Hamiltonian of the two-dimensional $q=8$ state Potts model is

$$\mathcal{H}=-J\sum_{\langle ij\rangle}\delta_{\sigma_i\sigma_j}\ ,$$

where J is the interaction constant, the sums run over distinct nearest-neighbor pairs on a square lattice, and the N spins can take on values of $\sigma_i=1,2,\ldots,8$. The system is quenched from infinite temperature to a low temperature T. Following the quench, the system evolves by spin-flip dynamics: The state of a randomly selected spin is changed to another randomly selected state if there is no increase in energy, or with probability $e^{-\Delta E/T}$, if the exchange increases the lattice energy by ΔE, where Boltzmann's constant has been set to unity. Fig. 1 shows some typical configurations as the domains grow.

Lattices of size $N=256^2$ and 128^2 were simulated at $T/J=0.6$ and $T=0$ using periodic boundary conditions. The results for the smaller system, which we studied over 5000 Monte Carlo steps (MCS), were averaged over 64 independent runs. On the larger lattice, results are averaged over 45 runs. The average domain size $R(t)$ was monitored in two different ways: from the inverse perimeter density and by monitoring the number of vertices in the evolving system. The inverse perimeter system density $R_p(t)$ is

$$R_p(t)=\left[3-\left\langle \frac{1}{N}\sum_{\langle i,j\rangle}\delta_{\sigma_i,\sigma_j}\right\rangle\right]^{-1},$$

where the angular brackets denote an ensemble average. The average area density

$$R_A(t)=\langle A(t)/\pi\rangle^{1/2}$$

was found using Euler's formula for a finite system:[6] $N_d-N_e+N_v=1$, where N_d is the number of domains, N_e the number of edges, and N_v the number of vertices, respectively. Since every vertex is three rayed on a triangular lattice, this implies that $2N_e=3N_v$ so that $N_d=N_v/2$. The mean area on the triangular lattice is therefore related to the total area A_T by $\langle A(t)\rangle=2A_T/N_v(t)$. The length scales $R_p(t)$ and $R_A(t)$ were sampled every 10 MCS. For both measures of domain size, we calculated the variance from the fluctuations of each run: $\Delta R(t)=(\langle R^2\rangle-\langle R\rangle^2)^{1/2}$. From this, the estimated statistical error δR was taken to be $\delta R=\Delta R(t)/\sqrt{\mathcal{N}-1}$, where $\mathcal{N}$ is the number of independent runs.

We used the renormalization group to exploit the scale invariance of the evolving system: The system is invariant, provided we rescale both length and time appropriately. The relationship between these rescalings is implicit in the growth law. The renormalized lattices were obtained by a block-spin transformation, with length rescaling factor $b=2$. The majority-rule transformation was used to generate new cell spin variables from the original spin configurations. There one chooses a renormalized spin from a block of b^d spins by letting the spins vote, and the majority rule. "Ties" were broken by randomly assigning a state to the block spins. Figure 2 shows some typical results. The transformation explicitly renormalizes the domains and the moving interfaces between them. It iterates away behavior on short length scales,

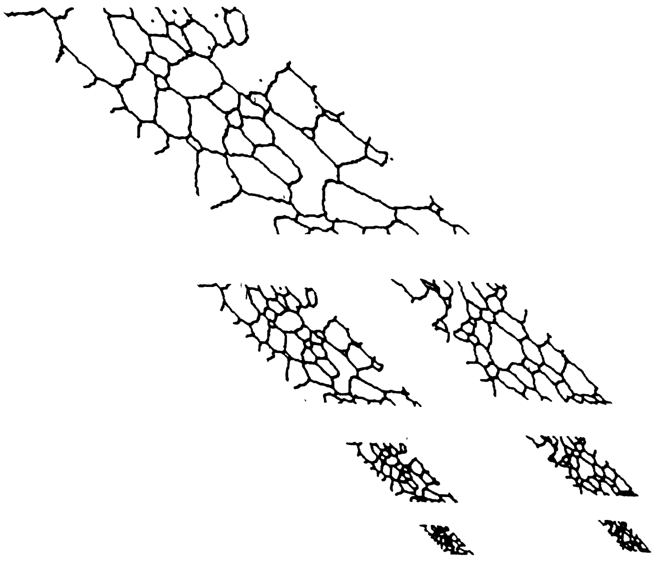

FIG. 2. Configurations on the left for $N=256^2$ system as it is renormalized at $t=4000$ MCS. Configurations on the right for $N=128^2$ system at $t=1000$ MCS as they are renormalized. Note the similarity between configurations as they are renormalized, with this choice of time rescaling factor ($n=\frac{1}{2}$).

thus permitting the investigation of the asymptotic large-length-scale properties of the system.

The growth law is determined by a matching procedure. In principle, after the irrelevant variables have been iterated away, the probability distribution function will remain invariant under further renormalization-group transformations. It is expected that, after a finite number of iterations, contributions from the irrelevant variables will be negligible. Then, any quantity determined after m blockings of an N spin system should be identical to those determined after $m+1$ blockings of a system of Nb^d spins. However, since the larger lattice has been renormalized once more, quantities will be at different times t and t'. Figure 2 shows this for some typical configurations. Hence, close to the fixed point, one can expect a matching condition to hold:

$$R(N,m,t)=R(Nb^d,m+1,t') .$$

From this the time rescaling factor t'/t can be calculated, and the growth exponent can be obtained, since

$$\frac{t'}{t}=b^{1/n} .$$

To ensure that the renormalized quantities are consistent with each other, one must check that scaling occurs for more than one iteration of the block-spin transformation.

The numerical value of the growth exponent n is the signature of the mechanism driving phase separation. During the late stages of domain growth the system is in a far-from-equilibrium state with many interfaces and thus a large amount of surface free energy. The system decreases its free energy as domains of ordered phase grow. If the order parameter is nonconserved, then the interfacial motion acts to reduce local surface area;

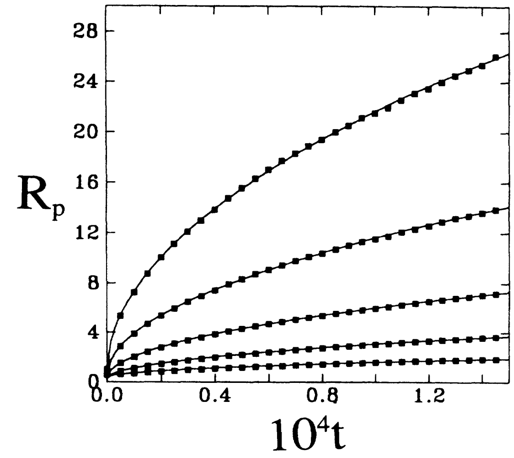

FIG. 3. $R_p(t)$ vs time. Starting at the top, the data for the $m=0$, 1, 2, 3, and 4 iterations of the renormalization-group transformation are shown. The solid lines show the best fit of the data to $R(t)=A+Bt^{1/2}$.

curved interfaces move, and when part of an interface becomes flat, it stops moving. For $q=2$, the interface velocity is then determined by the well-known Allen-Cahn law,[2,3] which leads to an $R(t)\sim t^{1/2}$ growth law.

We first looked for the best fits to the renormalized data. Figure 3 shows that the R_p data, at all levels of renormalization down to $m=3$, can be fit exceedingly well by $R_p(t)=A+Bt^{1/2}$. In contrast, before renormalization, the R_A data were fitted better by $n=\frac{1}{4}$ than $n=\frac{1}{2}$. See Fig. 4. Note that the data are fairly noisy for $m=0$, and that after renormalization the data are significantly smoother and fit $n=\frac{1}{2}$ better than $n=\frac{1}{4}$. The implica-

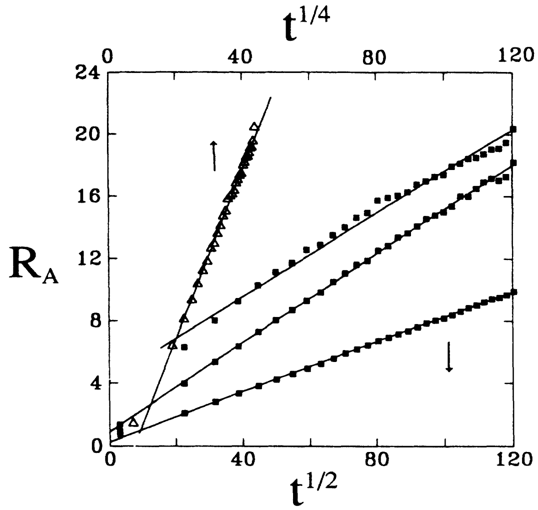

FIG. 4. $R_A(t)$ vs either $t^{1/4}$ or $t^{1/2}$. Open triangles show $m=0$ data vs $t^{1/4}$. The solid squares show R_A vs $t^{1/2}$ for $m=0$, 1, and 2 iterations of the renormalization-group transformation, from top to bottom. Solid lines show best fits. Note that $m=0$ data fit better to $t^{1/4}$ than $t^{1/2}$, indicating the presence of a transient, which is iterated away by the renormalization-group transformation.

TABLE I. Results of forced matching for R_p. The first value of R_p has had the renormalization group applied to it one less time than the value beneath it. Percent error is quoted.

Time	$m=0,1$ R_p	Error	$m=1,2$ R_p	Error	$m=2,3$ R_p	Error
10	1.008	−5.43	0.731	2.71	0.624	−0.92
	1.066		0.712		0.630	
100	2.646	1.32	1.483	5.21	0.872	3.70
	2.611		1.410		0.841	
500	5.332	−1.20	2.881	2.36	1.543	3.57
	5.398		2.815		1.489	
600	5.806	−1.02	3.125	2.40	1.659	3.18
	5.866		3.051		1.608	
700	6.225	−1.12	3.351	2.64	1.773	3.49
	6.295		3.264		1.713	
800	6.618	−0.94	3.550	2.30	1.878	3.61
	6.680		3.470		1.812	
900	6.975	−1.32	3.743	1.93	1.972	3.10
	7.070		3.647		1.913	
1000	7.302	−2.10	3.919	1.29	2.066	2.71
	7.456		3.869		2.011	
1100	7.637	−2.20	4.104	1.15	2.157	2.43
	7.809		4.056		2.106	
1200	7.971	−2.90	4.269	0.60	2.250	1.69
	8.210		4.243		2.213	

tion is that there exists a strong transient with an effective exponent of $n \approx \frac{1}{4}$, to which R_A is sensitive. While we fitted our data for $R_A(t)$ to $n=\frac{1}{4}$, we cannot rule out other numerical values for the transient growth exponent; this choice is based on a tentative identification of the transient with the effective exponent seen in systems with "soft" walls.[7,22] For early times, transients due to the structure of the walls will be more important, and the growth will resemble that in soft-wall systems.

Our estimate for n was obtained by determining the ratio of times, on two lattices at different levels of renormalization, which gave equal domain sizes. The estimates of n from four levels of matching are 0.51, 0.48, 0.47, and 0.48, respectively. Averaging these gives an estimate of the growth exponent of 0.48 ± 0.04, which is consistent with the expected value of $\frac{1}{2}$. We also assumed $n=\frac{1}{2}$, and checked whether R's at different levels of renormalization approached each other. The results, which are again consistent, with $n=\frac{1}{2}$, are presented in Table I for R_p, and Table II for R_A. The large transient mentioned above is evident from inspection of Table II.

B. Structure factor and edge distribution function

The structure factor $s(\mathbf{k},t)$ was calculated as follows: For a given lattice configuration, we set all of the sites of a given Potts state to unity, and the rest of the sites to -1. The Fourier transform was then taken. This procedure was then repeated for all of the Potts states of the system, and the results were then averaged; i.e.,

$$s(\mathbf{k},t) \equiv \left\langle \frac{1}{N} \left[\sum_{\mathbf{r}_i} \frac{1}{q} \sum_{i=1}^{q} (2\delta_{\sigma(\mathbf{r}_i,t),i} - 1) e^{i\mathbf{k}\cdot\mathbf{r}_i} \right]^2 \right\rangle ,$$

where $\mathbf{r}_i$ is a vector on the triangular lattice, and $\mathbf{k}=(2\pi/L)(m\mathbf{b}_1+n\mathbf{b}_2)$ with $m,n=1,2,\ldots,L$, where L is the system size and $\mathbf{b}_1$ and $\mathbf{b}_2$ are the reciprocal lattice vectors. A spherical average then gives the circularly averaged structure factor $S(k,t)$. As the domain growth proceeds, the system builds up a Bragg peak which narrows with time about the $k=0$ mode. The results presented are averaged over only three independent quenches for a lattice of size $N=256^2$, and so are fairly noisy. For late times, all length scales have their time dependence set by the size of growing domains. Thus the dimensionless pair-correlation function satisfies $g(r,t) \sim G(r/R(t))$, which implies that its Fourier transform,

$$S(k,t)=R^d(t)F(x) ,$$

where $x=kR(t)$. For any given level of renormalization, scaling with R_p appears to hold, provided that $t \geq 200$ MCS. To investigate the scaling of $S(k,t)$ in a more

TABLE II. Results of forced matching of R_A. The first value of R_A has had the renormalization-group transformation applied to it one less time than the value below it. Percent error is quoted.

Time	$m=0,1$ R_p	Error	$m=1,2$ R_A	Error	$m=2,3$ R_A	Error
10	1.400	−5.80	0.972	4.98	0.788	−1.16
	1.4868		0.925		0.797	
100	3.460	−3.63	2.680	9.12	1.166	6.14
	3.590		1.906		1.098	
500	6.276	−13.78	3.988	4.00	2.105	5.66
	7.279		3.834		1.992	
600	6.741	−14.91	4.300	3.30	2.257	5.176
	7.923		4.160		2.146	
700	7.114	−15.64	4.595	3.24	2.417	5.24
	8.43		4.451		2.296	
800	7.486	−16.01	4.878	3.28	2.561	6.08
	8.920		4.723		2.414	
900	7.848	−16.81	5.143	2.38	2.685	4.44
	9.434		5.023		2.571	
1000	8.094	−18.34	5.346	1.39	2.813	4.51
	9.912		5.273		2.692	
1100	8.323	−19.14	5.605	1.08	2.948	3.96
	10.284		5.545		2.835	
1200	8.678	−20.72	5.820	−0.68	3.068	3.68
	10.937		5.860		2.959	

qualitative fashion, $F(x)$ was fit to the expression derived by Ohta, Jasnow, and Kawasaki[3] for the Ising model. Figure 5 shows that our data are consistent with their result, although we do not have enough resolution at small x to test the form. More detailed tests of scaling have been given by Kumar *et al.*[9]

In Fig. 6, we show our results for the edge number distribution function $P(N_e)$, where N_e is the number of edges. We found that in the scaling regime, $t \geq 200$ MCS, the distribution is time invariant to the accuracy of our simulations after one iteration of the renormalization

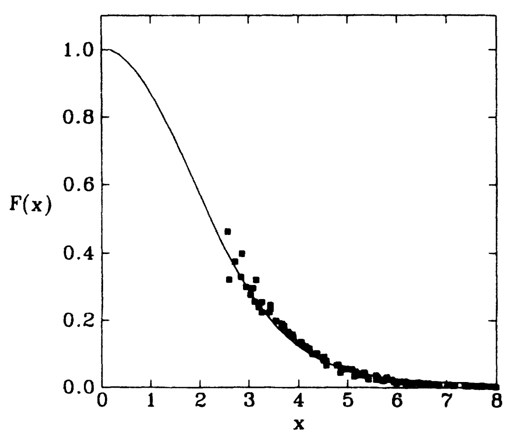

FIG. 5. Scaling function $F(x)$ vs scaled wave number $x=kR_p$, for $m=0$. Solid line is fit to Ohta-Jasnow-Kawasaki form. Times greater than 200 MCS are shown.

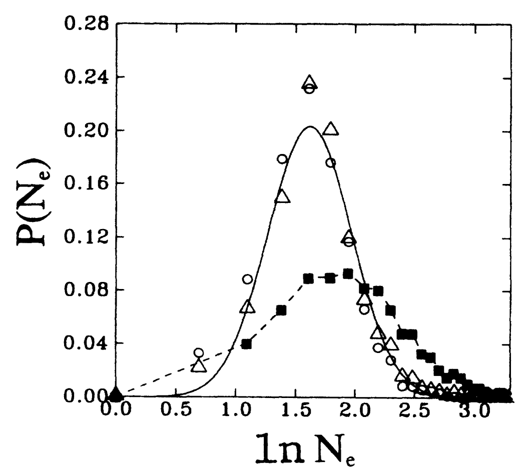

FIG. 6. Edge distribution function P vs natural logarithm of number of edges N_e. Form is approximately log symmetric. Solid squares connected by dashed line are $m=0$ data with thermal fluctuations removed; open triangles and open circles are $m=1$ and 2 data, respectively. Solid line is Gaussian fit to $m=1$ and 2 data.

group. The unrenormalized data are heavily skewed by thermal fluctuations of domains of one site, which have three edges. Renormalization removes these single-site domains, giving a distribution which remains approximately invariant under the application of the renormalization-group transformation. The functional form of the edge number distribution function is approximately log symmetric, with an average value of five edges per domain. We have also fitted to a log-Gaussian form in Fig. 6, following other work,[6,7,10,11] as a guide to the eye; the data are not of sufficient quality to estimate the form of the distribution.

C. Summary

In conclusion, quantities such as n and F have been obtained by MCRG, which proved to be a computationally efficient way to study domain growth in the presence of strong transients. The growth exponent was estimated to be $n = 0.48 \pm 0.04$, although we saw evidence of a transient which gives rise to growth exponents considerably smaller than $\frac{1}{2}$. The transient was tentatively identified with an effective exponent for domain growth with "soft" walls. We also obtained the scaled structure factor and the edge distribution function. Both the growth exponent and the scaling function agree with results for $q = 2$, the universality class of the nonconserved Ising model, which is consistent with these being superuniversal quantities, as has been previously suggested.[9]

Finally, it is worth noting that while our results are consistent with previous studies and provide further insight into the problem, unfortunately they do not represent a dramatic improvement over previous work. This raises the issue of how to improve MCRG for dynamical problems. We hope to return to this problem at a later time.

ACKNOWLEDGMENTS

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