Monte Carlo Renormalization-Group Study of the Dynamics of an Unstable State

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The kinetics of an order-disorder transition is studied by Monte Carlo renormalization-group methods. The block-spin transformation acts to renormalize both the growing domains and the moving interfaces separating them. After several iterations, the growth is found to be self-similar under a simultaneous rescaling of space and time. The growth law for the average size of domains is then determined by a matching condition. Good agreement with the results of previous studies is obtained.

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The Monte Carlo renormalization-group method has proved useful in the study of second-order phase transitions.[1-6] It was originally introduced by Ma,[1] and then developed and extended by Swendsen[3] and other workers[4] to a variety of equilibrium problems. Tobochink, Sarker, and Cordery,[4] and others,[5,6] have used the technique to study dynamical critical behavior. Their method, which we will extend below, involves matching correlation functions on different sized lattices at different levels of renormalization. Near the second-order transition, matching determines the dynamical critical exponent. We should note, however, that the usefulness of Monte Carlo renormalization-group methods for those problems remains controversial, as a result of the lack of an exact nontrivial result to test the method.

A related problem where a renormalization-group approach could be useful is the far-from-equilibrium dynamics of pattern formation in a first-order phase transition.[7-11] There, following a rapid quench from a disordered state to a low temperature, domains form which grow as time evolves. Experiments[9] and computer simulations[10] find that the growth process involves a characteristic time-dependent length, the average size of domains $\bar{R}(t)$, to which the spatial dependence of quantities scales. Furthermore, $\bar{R}$ often satisfies (at least approximately) a power-law form, $\bar{R}(t) \sim t^n$.

While these results are quite reminiscent of critical phenomena, it has not been possible to develop a first-principles renormalization-group approach for this class of problems to date. To our knowledge, the first attempt was by Langer and Bar-on[12] who studied spinodal decomposition. Later, Kawasaki[13] studied the scaling solution of the Allen-Cahn equation for interfacial dynamics, where the scalar order parameter is nonconserved. By far, the most successful approach using renormalization-group ideas, however, has been given recently in a series of papers by Mazenko and Valls.[8] They do not consider a Wilson-type renormalization group. Instead they consider the behavior of finite-size systems embedded in an "infinite" lattice. Monte Carlo simulations are then used both to verify a scaling relation for the average domain size and to determine the time rescaling factor defined through this relation. Then, they iteratively solve a recursion relation for the structure factor which they have proposed, using the time rescaling factor previously calculated. They find their results to be in reasonable agreement with Monte Carlo simulations. Given the success of their analysis, it is of interest to carry out an explicit standard application of a Wilson renormalization group.

In this Letter, we extend the Monte Carlo renormalization-group approach[1-6] to study the far-from-equilibrium kinetics of pattern formation in a first-order phase transition. In contrast to critical dynamics, here there is a well-established result in the literature which serves to check the validity, self-consistency, and accuracy of the method, that being $n = \frac{1}{2}$ for the nonconserved Ising model. Consequently, we consider here the kinetic Ising ferromagnet with spin-flip dynamics in dimension $d = 2$. The block-spin transformation, which explicitly renormalizes the domains as well as the moving interfaces, is used to obtain the growth exponent n. Our result, $n \cong 0.500$, is in agreement with previous theoretical,[11] experimental,[9] and computer simulation[10] studies. This shows that a block-spin renormalization group can be used to study this class of far-from-equilibrium problems.

It is clear from Fig. 1 that, after renormalization, the system is similar to itself at an earlier time. This is the familiar self-similarity seen in evolving phase-separating systems[7]: The system is approximately invariant under a change of length scales, given a corresponding change in time scales. The relationship between both is the growth law.

This is the scale invariance which we will exploit by the renormalization-group transformation. Before we discuss our treatment in detail, it is useful to discuss the flow of coupling constants under renormalization. Here we follow the description of Mazenko and Valls.[8] After m renormalizations, two sets of coupling constants, $K_i^{(m)}$ and $K_f^{(m)}$, characterize the equilibrium states at times $t = 0$ and $t = \infty$, respectively. Since we quench from above the critical point to below, the

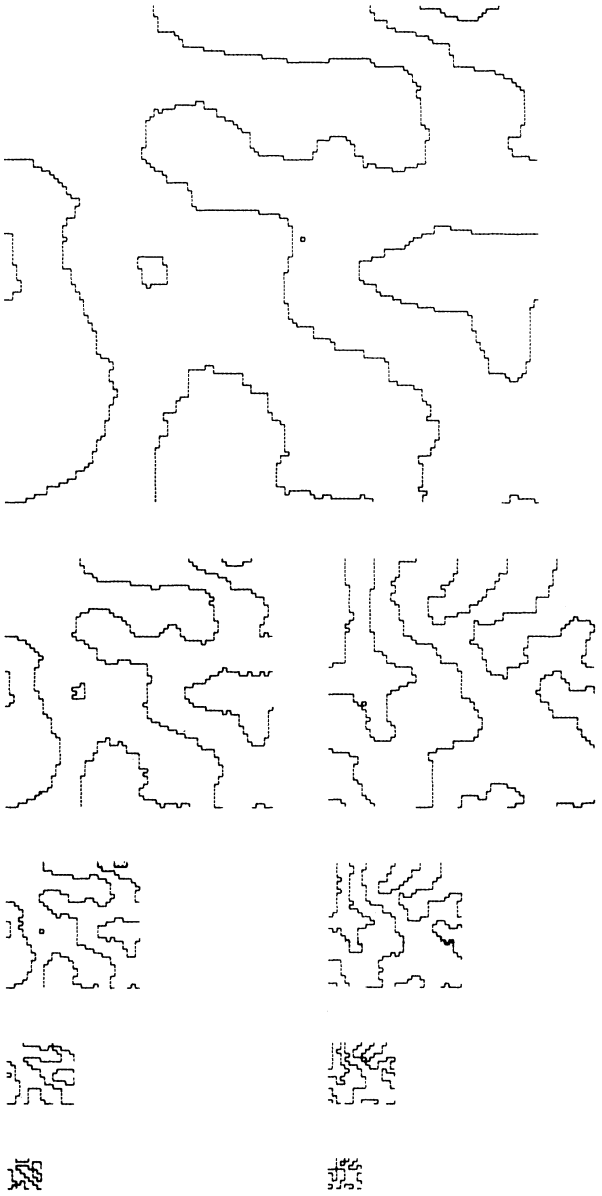

FIG. 1. The spin configurations on the left-hand side show the $N=128^2$ system being renormalized at time $t=100$ Monte Carlo steps. On the right-hand side, configurations for the $N=64^2$ system, as it is renormalized, are shown for $t=25$ Monte Carlo steps.

direction of flow as m increases is evident: The initial coupling constants will eventually flow to the trivial infinite-temperature fixed point, while the final coupling constants will flow to the trivial fixed point at zero temperature. That is, as $m\rightarrow\infty$, we would obtain $K_i^*=0$ and $K_f^*=\infty$. Thus, in contrast to critical phenomena, the dynamics here involves stable, attractive fixed points. While the Hamiltonian of the system is driven to the low-temperature fixed point, we note that, also, as $m\rightarrow\infty$ the renormalized time $t^{(m)}\rightarrow 0$. Roughly speaking, the renormalization-group transformation takes the system back to the initial condition, as can be seen in the results obtained for the average domain size. Thus, the asymptotic scaling regime involves time in a nontrivial way. Also, because of the flow of coupling constants the thermal correlation length ξ will be an irrelevant variable, in marked contrast to critical phenomena. Since $\xi\rightarrow 0$ under renormalization, the motion of the system simplifies to that of a more idealized system: the dynamics of very thin independent interfaces.

We now give a detailed description of our analysis. The reduced Hamiltonian for the two-dimensional Ising model is $H=-K\sum_{\langle ij\rangle}\sigma_i\sigma_j$, where the sum runs over distinct nearest-neighbor pairs and the N spins can take the values $\sigma_i=\pm 1$. After a quench from infinite temperature to low temperature K_f^{-1}, the system evolves by the standard Metropolis spin-flip Monte Carlo procedure. The unit of time is a Monte Carlo step which consists of N random attempts to update spins. The average size of domains (measured as the inverse perimeter density) is $\bar{R}(t)=2/(2+\epsilon)$, where $\epsilon=-(1/N)\langle\sum_{\langle ij\rangle}\sigma_i\sigma_j\rangle$. The unrenormalized $m=0$ systems consist of lattices of size $N=64^2$ (at temperatures $K_f^{-1}=0.75$ and 0.9), and $N=128^2$ (at $K_f^{-1}=1$).[14] To obtain the best possible statistics, 1000 runs were done at each of the temperatures for the 64^2 system and 750 for the 128^2 system. In studies of this kind,[10] finite-size effects become apparent for $\bar{R}\gtrsim 0.4\sqrt{N}$. Thus our results are based on the first 400 Monte Carlo steps for the $N=128^2$ system and the first 100 Monte Carlo steps for the $N=64^2$ system.

Renormalized lattices were obtained by majority-rule block-spin transformation of the evolving spin configurations. "Ties" were broken by randomly assigning block spins the value ± 1. The typical results of blocking, in groups of four spins is shown in Fig. 1. After m renormalizations there are Nb^{-md} block spins on the new lattice, where the length rescaling factor is chosen to be $b=2$. To obtain the growth law we have extended the matching procedure used by Tobochnik, Sarker, and Cordery[4] for critical dynamics. In principle, after the irrelevant variables have been iterated away, the probability distribution will remain invariant under the renormalization-group transformation. It is expected, then, that after a finite number of iterations (say m) the irrelevant variables will have essentially disappeared. Thus, any quantity determined after m blockings of N spins will be identical to that determined after $m+1$ blockings of Nb^d spins. However, since the time scale in the bigger lattice has been renormalized once more all quantities will be at different times t and t': $\bar{R}(N,m,t)=\bar{R}(Nb^d,m+1,t')$. This is the matching condition. The ratio of the times, t'/t,

give the time rescaling factor, $b^{1/n}$, resulting from the length rescaling b given by the renormalization group. Thus, by matching we can determine the growth law. We note that it is essential that matching occurs for more than one value of m to ensure that the renormalized probability distributions, $\rho(m)$ and $\rho(m+1)$, are tracking each other.[15]

The exponent n can now be estimated by requiring precise matching, i.e., by considering a given time on one lattice and then finding the time on the other lattice with the same value of $\bar{R}$. It is essential that the exponent obtained remains stationary after iteration. This is the case here after the first level of renormalization. The next three levels give essentially the same value for n, which is a direct consequence of the scale invariance of the system under the simultaneous rescaling of space and time. The results we obtain from estimating the exponent in this manner are 0.510, 0.497, and 0.501 (for $K_f^{-1}=0.90$), and 0.499, 0.492, and 0.499 (for $K_f^{-1}=0.75$). The average of these values is[16] $n=0.500\pm0.015$ which is in agreement with the results of many other studies.[9-11] The fifth matching is bad because the systems have only 4^2 block spins (so finite-size effects become important or, possibly, there is statistical error after many blockings).[17]

If now we assume that $n=\frac{1}{2}$ exactly, we obtain the results given in Table I. There we compare the value of $\bar{R}$ on the $N=128^2$ system after $(m+1)$ blockings at time $tb^{1/0.5}$ to the value on the smaller lattice after m blockings and at time t. This is done to show, explicitly, the result of the renormalization-group transformation. We again see there how the matching is bad after the first level improves, and is reasonably good during three more iterations. We have two additional remarks on the matching. For late times, $t>80$ Monte Carlo steps for the $N=64^2$ system, the matching gets worse, which is a finite-size effect. We also note that, even though the matching we obtain is quite reasonable, we have not reached the limiting behavior

TABLE I. We compare the value of $\bar{R}(tb^2)$ for the 128^2 system every tenth Monte Carlo step (we have data for every five Monte Carlo steps) and at different levels of renormalization (denoted K_m) to the value of $\bar{R}(t)$ for the 64^2 system at levels K_{m+1}. The two different temperatures studied for the 64^2 system are written, top to bottom at a given time, $K^{-1}=0.9$ and 0.75, respectively. The percentage mismatch is shown, and given a sign. The estimated error in the data for $\bar{R}$ is less than 1%.

Time	$\bar{R}^2(K_1)$	$\bar{R}^2(K_0)$	%	$\bar{R}^2(K_2)$	$\bar{R}^2(K_1)$	%	$\bar{R}^2(K_3)$	$\bar{R}^2(K_2)$	%	$\bar{R}^2(K_4)$	$\bar{R}^2(K_3)$	%	$\bar{R}^2(K_5)$	$\bar{R}^2(K_4)$	%
10	26.470	28.304	6.9	7.609	7.572	-0.5	2.528	2.610	3.3	1.342	1.355	1.0	1.167	1.079	-7.5
		29.618	11.9		7.720	1.5		2.601	2.9		1.344	0.1		1.083	-7.2
20	51.867	57.077	10.0	14.371	14.277	-0.7	4.215	4.332	2.8	1.723	1.718	-0.2	1.218	1.176	-3.4
		59.707	15.1		14.463	0.6		4.318	2.5		1.718	-0.2		1.169	-4.0
30	77.112	85.114	10.4	21.211	20.876	-1.6	5.955	6.067	1.9	2.136	2.137	0.0	1.311	1.262	-3.7
		89.878	16.6		21.206	0.0		6.102	2.5		2.138	0.1		1.223	-6.7
40	101.965	113.447	11.3	27.833	27.472	-1.3	7.662	7.796	1.8	2.544	2.581	1.5	1.445	1.327	-8.2
		120.150	17.8		28.072	0.9		7.859	2.6		2.560	0.7		1.311	-9.3
50	127.168	140.641	10.6	34.706	34.032	-1.9	9.402	9.543	1.5	2.952	2.990	1.3	1.512	1.397	-7.6
		150.690	18.5		34.921	0.6		9.680	3.0		3.011	2.0		1.406	-7.0
60	152.520	168.434	10.4	41.380	40.451	-2.2	11.166	11.255	0.8	3.372	3.420	1.4	1.607	1.527	-5.0
		181.911	19.3		41.933	1.3		11.531	3.3		3.480	3.2		1.504	-6.4
70	177.566	195.523	10.1	48.190	46.987	-2.5	12.989	12.952	-0.3	3.828	3.810	-0.5	1.754	1.599	-8.8
		212.687	19.8		48.706	1.1		13.307	2.4		3.889	1.6		1.627	-7.2
80	203.777	222.867	9.4	55.179	53.205	-3.6	14.837	14.529	-2.1	4.347	4.239	-2.5	1.842	1.686	-8.5
		242.927	19.2		55.509	0.6		15.072	1.6		4.326	-0.5		1.703	-7.6

governed by the stable fixed points, $K_i^* = 0$ and $K_f^* = \infty$. This is because $\bar{R}$ for the two $N = 64^2$ systems (with quench temperatures $K_f^{-1} = 0.75$ and 0.9) should become identical there. Clearly, however, we are quite close to that limiting behavior since we obtain good matching. Compare, also, the two values of $\bar{R}$ for the $N = 64^2$ system as we renormalize, at a given time, in Table I.

Our results indicate that Wilson's first-principles renormalization group, as implemented by Monte Carlo renormalization-group methods, can be applied to study the decay of unstable states in first-order phase transitions. Our work has not indicated any major difficulties with the method, other than the need for very accurate statistics and care in interpretation of the results. The method can be straightforwardly modified to study other lattice-gas models with nonconserved dynamics. In the future, we intend to apply this method to obtain the scaling form of the structure factor and to study the related problem of spinodal decomposition.

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[14]We have chosen different quench temperatures to check that the quench temperature is irrelevant, i.e., that $K_f^{(m)} \to \infty$.

[15]The crucial assumption in all Monte Carlo renormalization-group studies is that one can iterate away the irrelevant variables. Here, since it is well established that $n = \frac{1}{2}$, the self-consistency of our Monte Carlo renormalization-group approach can be seen from the relatively rapid convergence to this value.

[16]The error bars are based on the uncertainty in the data for $\bar{R}$, and the uncertainty due to the linear interpolation of the discrete time used to obtain the values.

[17]We have tested the goodness of the fit $\bar{R}^2(m,t) = a + bt$ after m blockings. The fit is good for $m = 0$, improves for $m = 1$ and $m = 2$, and is slightly worse for $m = 3$ and $m = 4$.