Fixed points and domain growth for the Potts model

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We present a Monte Carlo renormalization-group analysis of the dynamics of the eight-state Potts model with nearest- and next-nearest-neighbor interactions after a quench below its phase-transition point. Our results suggest the existence of at least two distinct fixed points at zero temperature. One is associated with a freezing behavior while the second is associated with equilibration. Our conclusion is that the freezing fixed point is only attractive for quenches to zero temperature, while the equilibration fixed point is attractive for quenches to finite temperature.

Renormalization-group ideas have been recently applied to study the far-from-equilibrium dynamics of a system following a quench from a high-temperature, disordered state to a low-temperature, unstable state below T_c.[1-4] (In what follows T_c denotes either a first- or second-order phase-transition point). Following such a quench, domains form and grow with time. Often the time dependence of the average domain size $\bar{R}(t)$ can be characterized by a power-law or logarithmic behavior (as in critical phenomena), $\bar{R}(t) \sim t^n$. (In many cases studied so far, however, it is quite possible that the reported values of n represent effective exponents rather than an asymptotic growth law.) It has also been observed in experimental[5] or computer simulation studies[6,7] that a nonequilibrium, dynamical scaling holds, with quantities such as the scattering intensity scaling with respect to a characteristic length, such as $\bar{R}(t)$.[8]

These renormalization-group studies have suggested that the nonequilibrium dynamics of the system is governed by its zero-temperature fixed-point structure. In the two cases studied so far[3,4] (the nearest-neighbor Ising ferromagnet with Glauber dynamics and Kawasaki dynamics, respectively), only one zero-temperature fixed point has been determined for each system. In the nonconserved case (the Glauber model), the system equilibrates at zero temperature and its behavior near the zero-temperature fixed point leads to the result predicted by Allen and Cahn and others, namely, $n=\frac{1}{2}$ for all $T<T_c$.[9] The physical origin of this growth law is curvature-driven interface motion. In the conserved case (the Kawasaki model), however, the system freezes at zero temperature, rather than equilibrating. Mazenko and Valls[3] have recently applied renormalization-group ideas and Monte Carlo calculations to argue that the zero-temperature fixed point associated with this freezing behavior leads to a logarithmic growth law for sufficiently low quench temperatures. The physical argument given for this growth law is that diffusion across an interface at low temperature is an activated process, with an activation energy which is inversely proportional to the local curvature. (They also argue that the Lifshitz-Slyozov theory[10] is incorrect for solids, based on their recent Monte Carlo work.) Thus, an important theoretical issue is the nature and influence of zero-temperature fixed points in nonequilibrium dynamics. This is particularly true given that no analytical theory of this subject is available at present.

In this article, we report for the first time evidence for the existence of at least two zero-temperature fixed points in the same system, one associated with freezing and one associated with equilibration. We analyze the ferromagnetic Q-state Potts model (with $Q=8$) on a square lattice, with both nearest- and next-nearest-neighbor interactions using a recently developed Monte Carlo renormalization-group (RG) technique.[4]

When the system is quenched to zero temperature, our study shows that the stable fixed point is the one associated with freezing. Only for the special case in which the initial nearest- (NN) and next-nearest-neighbor (NNN) interaction constants are equal do we find that the equilibration fixed point is attractive at zero temperature. (The unfreezing of the square lattice at $T_f=0$ for this special case was first pointed out in an earlier Monte Carlo study of Sahni *et al.*[7]) Our results suggest that in this case the growth-law exponent is $n \simeq 0.48$, which is the same exponent found at finite temperature (by standard Monte Carlo simulation) for this model on both the triangular and square lattices.

When the system is quenched to a finite temperature, with any value of the original interaction constants,[11] it is also found to reach equilibrium. However, the existence of these two fixed points at zero temperature raises two important points about the dynamics of the Potts model on a square lattice at finite temperatures. The first point concerns the stability of the fixed points for finite-temperature quenches. We can envisage two possibilities: If the freezing fixed point were attractive, the asymptotic growth law would presumably be logarithmic.[12] As a consequence, the Potts model on the square and triangular lattices would belong to different universality classes [for the triangular lattice, Monte Carlo results indicate that $n(Q=8) \simeq 0.48$ for all temperatures $T_f \geq 0$]. The opposite possibility would simply imply that the growth law at finite temperature would be the same on both lattices. The second point is that, in any event, there should be a crossover behavior in the domain growth at finite temperatures due to the existence of two fixed points, as in critical phenomena. We elaborate further on these points in the conclusion, where we argue that the equilibration fixed point is attractive for the square lattice, so that both the triangular and square lattices would belong to the same universality class. We also note at this point that the analysis of any crossover effect, using Monte Carlo technique, is restricted to finite lattices. Consequently, it is not possible to unequivocally determine the late stage growth of an infinite system (although we believe the conclusions we present should hold for the infinite system). For that reason, we think that our results showing the existence of two fixed points establish the need for an analytical theory of this problem.

The details of our calculation are as follows. The Hamiltonian of the model is defined as

$$H=-J_{\rm NN}\sum_{\rm NN}\delta_{\sigma_i\sigma_j}-J_{\rm NNN}\sum_{\rm NNN}\delta_{\sigma_i\sigma_k} \qquad (1)$$

The system has been quenched from an initially disordered state ($T_i=\infty$) to different final temperatures $T_f/J_{\rm NN}$ from 0 to 0.6. We have also done a variety of quenches for different values of $J_{\rm NNN}/J_{\rm NN}$ ranging from 0 to 1.1. We use spin-flip dynamics (Metropolis rule) on several lattices of $N=128^2$, 64^2, and 32^2 spins, respectively. The average size of the domains is calculated from the nearest-neighbor correlation function: $\bar{R}(t)=(1/N)\langle\sum_{\rm NN}\delta_{\sigma_i\sigma_j}\rangle$ for a period of 10 000 Monte Carlo steps per spin (MCS) after the quench for the 64^2 and 32^2 lattices and 5000 MCS for the 128^2 lattice. In order to have reasonable statistics, the results have been averaged over a large number of quenches, ranging between 150 and 200 in the smaller lattices and between 80 and 160 in the 128^2 lattice. The configurations obtained are renormalized using a standard block transformation (with a rescaling factor $b=2$). The renormalized cell spins are obtained by a generalized majority rule, where ties are broken at random.

The main results of our calculation are shown in Figs. 1 and 2. We show there the average domain size as a function of time for quenches to zero and finite temperature. We include also the average domain size calculated after a few iterations of the RG transformation for the same temperatures and values of the interaction constants. The usual way to obtain the growth exponent by the Monte Carlo RG method involves invoking a matching condition between the average domain size calculated in two different lattices of the same size but at different levels of renormalization (see Ref. 4 for a detailed description): $\bar{R}(N,\ m,\ t)=\bar{R}(Nb^d,\ m+1,\ t')$. When the time rescaling $\Delta(T_f,t)=t'/t$ is constant, it gives the exponent n: $\Delta=b^{1/n}$. When the system is quenched to zero temperature with $J_{\rm NNN}/J_{\rm NN}\neq 1$, $\Delta(t)$ monotonically increases in time.[13] This indicates that the system is freezing at late times. This effect can also be seen by fitting an effective exponent at different intervals of time and different levels of renormalization. In all cases, it approaches zero, i.e., the system freezes (see Fig. 1). The change in the exponents after renormalization, as well as a similar freezing behavior observed for values of $J_{\rm NNN}$ close to but different from $J_{\rm NN}$, indicate that the freezing point is stable when the system is quenched to zero temperature. In the special case where $J_{\rm NNN}/J_{\rm NN}=1$, the system equilibrates with a growth law given by $n\simeq 0.48$.

In Fig. 3 we show typical configurations obtained when

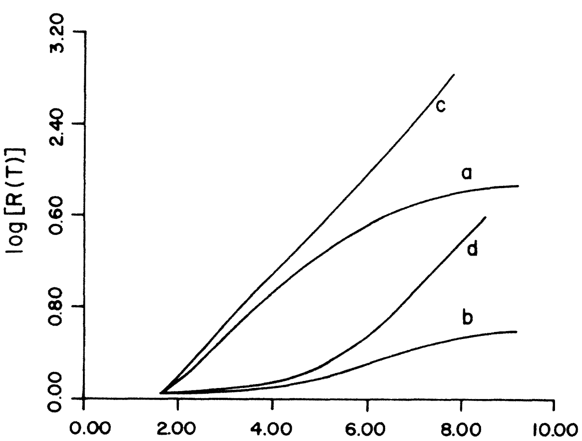

FIG. 1. Average domain size as a function of time (MCS in the unrenormalized lattice) for quenches to $T_f=0$ and (a) $J_{\rm NNN}/J_{\rm NN}=0$, original lattice; (b) $J_{\rm NNN}/J_{\rm NN}=0$, after 3 renormalizations; (c) $J_{\rm NNN}/J_{\rm NN}=1$, original lattice; and (d) $J_{\rm NNN}/J_{\rm NN}=1$, after 3 renormalizations. Each curve has been multiplied by an arbitrary factor to fit them all in the same figure. The slope of each curve gives the effective exponent n.

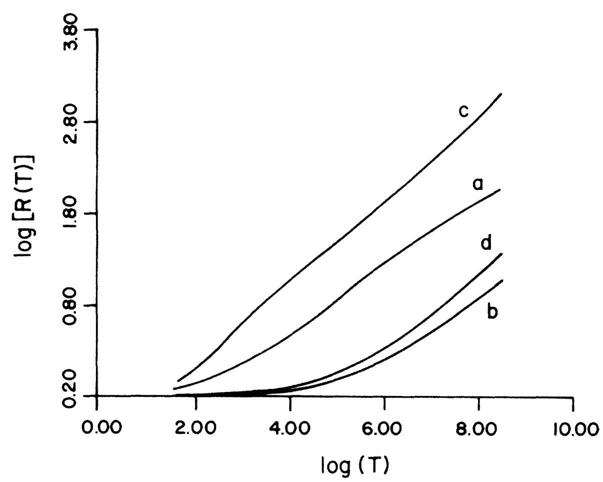

FIG. 2. The same as in Fig. 1, but here the quench temperature is $T_f/J_{\rm NN}=0.6$.

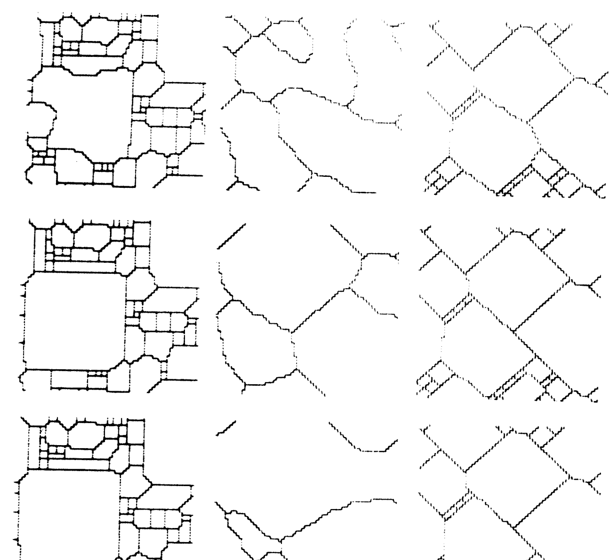

FIG. 3. From left to right, typical configurations for $J_{\rm NNN}/J_{\rm NN}=0.9$, 1, and 1.1 after 1000, 3000, and 5000 MCS after the quench to zero temperature (top to bottom).

the system is quenched to zero temperature for $J_{NNN}/J_{NN}=0.9$, 1.0, and 1.1 for times 1000, 3000, and 5000 MCS, respectively, after the quench. The freezing that occurs for 0.9 and 1.1 is evident, whereas the system with $J_{NNN}/J_{NN}=1$ easily equilibrates. The change in the topology of the domains is also clear: For $J_{NNN}/J_{NN}<1$, horizontal and vertical walls are the only ones present at late times, whereas only flat diagonal walls are present for $J_{NNN}/J_{NN}>1$. Both cases reflect the underlying square symmetry of the dominant interaction and both show, at late times, flat walls which are correspondingly pinned at the vertices. The case $J_{NNN}/J_{NN}=1$ corresponds to a degenerate situation. The microscopic picture underlying these results is, schematically, the following. For $J_{NNN}/J_{NN}<1$ kinks are absorbed at square vertices which are, in turn, pinned.[14] At $J_{NNN}=J_{NN}$ kink generation is possible at vertices even at $T_f=0$.[7] This generation plus the existence of vertical or horizontal interfaces at the vertices ("square" vertices) allows them to move and, eventually, annihilate. At higher J_{NNN}, there is still kink generation at "square" vertices, but now diagonal flat walls are strongly preferred. Consequently, the vertices cannot move and the system is again pinned.

However, when the system is quenched to a finite temperature, it reaches equilibrium at long enough times. There are two distinctive time regimes as can be seen in Figs. 1 and 2. For early time and after enough iterations, one can obtain an effective exponent very close to zero indicating that the system has not yet reached the scaling regime. At later times, the growth is characterized by a finite exponent very close to the zero-temperature value for $J_{NNN}/J_{NN}=1$. The same value is obtained from a power-law fit to the corresponding average domain size or from the matching condition discussed above (as long as one stays within the time regime—different at each level of renormalization—where the system exhibits a power-law behavior).

Given these facts, we now return to the issue raised in the introduction as to which of the two fixed points is attractive for quenches to finite temperature. Our conclusion is that it is the equilibration fixed point which is attractive. This is entirely consistent with our observation that the system equilibrates at finite temperatures, with a growth law characterized by an exponent which is (within the precision of our study) the same as that of the equilibration fixed point at zero temperature. The alternative scenario (that the freezing fixed point is the attractive one) would imply that the system has an asymptotic growth law which is logarithmic. While we cannot completely rule out this possibility for an infinite system after a sufficiently long time (i.e., a crossover from $n\simeq0.48$ to logarithmic growth) we see no evidence for this crossover in our study. Additionally, on physical grounds, we have no reason to expect that an infinite system quenched to a finite temperature would have an asymptotic logarithmic growth law. For example, whereas at zero temperature one can fill the square lattice with square domains in local equilibrium, and hence pin the system, at finite temperatures the local equilibrium shape of domains is not a square (but circular) and so one cannot "tile" the two-dimensional system, pinning it in a metastable state.[15]

Thus, our interpretation of our results is that the freezing fixed point is unstable with respect to temperature and could play a role in the dynamics only at very low temperature and "early" times. Otherwise, the attractive fixed point is the zero-temperature equilibration fixed point discussed above. One can understand the crossover behavior heuristically as follows. If one imagines that the equilibration fixed point governs the dynamical behavior for times $t>\tau(T_f)$, where $\tau(T_f)$ is a temperature-dependent characteristic time, one knows that $\tau(T)\rightarrow\infty$ as $T\rightarrow0$. Thus, for quenches to very low temperature, one might not see the true domain growth in Monte Carlo studies unless one runs for very long times since $\tau(T)$ is very large. Thus we would speculate that the temperature-dependent exponent $n(T)$ at low temperatures found in the literature[7,16] is not the true growth exponent, but only an effective exponent related to the existence of the freezing fixed point.[17] If this is the case, the freezing fixed point would seem to be an artifact of the square lattice (or its topological equivalent) since it is known that the Potts model on a triangular lattice does not freeze. One would therefore find it difficult to obtain the true growth law for the square lattice at low temperature. In order to test these ideas, we have done additional preliminary quenches to $T_f/J_{NN}=0.1$ and 0.2, where the values quoted in the literature for the exponents markedly deviate from the value given here.[7,16] For $T_f/J_{NN}=0.2$, the system is seen to reach equilibrium after a very long time. This is consistent with the scenario outlined above. For $T_f/J_{NN}=0.1$, although the system has not yet equilibrated for the 30 000 MCS analyzed, we see no indication of freezing or logarithmic growth. A more detailed analysis of the low-temperature behavior will be presented elsewhere.

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