Nonequilibrium phase ordering with a global conservation law

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(Received 11 March 1996)

In all dimensions, infinite-range Kawasaki spin exchange in a quenched Ising model leads to an asymptotic length scale $L \sim (\rho t)^{1/2} \sim t^{1/3}$ at $T=0$ because the kinetic coefficient is renormalized by the broken-bond density, $\rho \sim L^{-1}$. For $T>0$, activated kinetics recovers the standard asymptotic growth law, $L \sim t^{1/2}$. However, at all temperatures, infinite-range energy transport is allowed by the spin-exchange dynamics. A better implementation of global conservation, the microcanonical Creutz algorithm, is well behaved and exhibits the standard nonconserved growth law, $L \sim t^{1/2}$, at all temperatures. [S1063-651X(96)11007-2]

PACS number(s): 05.70.Ln, 05.50.+q, 64.60.Cn

Globally conserved dynamics offers a useful test of our theoretical understanding of phase ordering [1] because it allows access to off-critical quenches without requiring diffusive ''model-B'' transport of the order-parameter. Renormalization group (RG) [2] arguments show that adding global conservation changes neither the critical dynamics nor the asymptotic growth law after a quench into the ordered phase. This has been confirmed by numerical studies [3]. The only change to nonconserved dynamics is to impose $\partial_t \langle \phi \rangle = 0$ where, using spin language, ϕ is the local magnetization ($\langle \phi \rangle$ is its spatial average). The standard ''model-A'' dissipative dynamics are $\partial_t \phi = -\Gamma \delta F / \delta \phi$, where $F[\{\phi\}] = \int d^d r [(\nabla \phi)^2 + (\phi^2-1)^2]$. The global constraint is imposed with a uniform magnetic field term, $H \langle \phi \rangle$, added to F. The field $H(t)$, effectively a Lagrange multiplier, is decreased smoothly while the ordering progresses so as to maintain $\langle \phi \rangle$ constant.

With a global conservation law, $\langle \phi \rangle$ is a tunable parameter that does not change the growth law but does affect scaled correlation functions and other aspects of the system. One can use this to explore what ''universality'' entails in nonequilibrium phase ordering systems. For example, with global conservation in Ising models, Sire and Majumdar [4] have shown that the autocorrelation exponent λ depends on the net magnetization. This author [5] has found spatial anisotropy in scalar phase ordering systems that depends strongly on $\langle \phi \rangle$.

However, there has been uncertainty about how to implement global conservation. Tuning a magnetic field to maintain $\langle \phi \rangle$ is impractical in computer simulations, due to the stochastic nature of most algorithms. Two alternative algorithms have been used for Ising models: a Creutz demon [6], and infinite-range Kawasaki spin exchange [3,4,7]. Differences between these two implementations at low temperatures has led to some confusion in the past [4,7,8]. In this report we clarify the situation.

For a two-dimensional Ising model on a square lattice, consider infinite-range Kawasaki exchange dynamics [3,4,7]: two randomly selected spins are exchanged under heat-bath dynamics, i.e., with probability $1/[1+\exp(\Delta E/k_B T)]$, where ΔE is the energy change under the spin exchange. The exchange satisfies global conservation. However, at low temperature the asymptotic dynamics are *activated*, and cross over to a different growth law at zero temperature.

At $T=0$, no exchanges that increase the energy are accepted. Starting from random initial conditions, aggregation of spins takes place and the broken-bond density $\rho(t)$ will be proportional to the domain wall density at late times, $\rho \sim L^{-1}$. Isolated spins with all bonds broken, of number density N, will aggregate rapidly onto existing domains, $\partial_t N \propto -\rho N$, and may be ignored. Spins that are part of domain walls can exchange, but only with the fraction ρ of the system that has broken bonds (i.e., that are also on domain walls). This rescales the effective kinetic coefficient by a factor of $\rho \sim L^{-1}$. For $T=0$ infinite-range Kawasaki exchange we thus expect $L \sim (\rho t)^{1/2} \sim (t/L)^{1/2} \sim t^{1/3}$, where $t^{1/2}$ is the standard nonconserved growth [1]. This applies in any dimension.

For $T>0$, thermal fluctuations provide partners for spin exchange and also allow exchange with bulk spins. These activated processes will dominate after the broken-bond density becomes comparable to the equilibrium average. After a quench, this will result in a crossover from intermediate $L \sim t^{1/3}$ growth to asymptotic $L \sim t^{1/2}$ growth. [The length scale is extracted from the scaling of the spherically averaged correlation function $C(r,t) = \langle \phi(x) \phi(x+r) \rangle = M^2 f(r/L)$, where M is the equilibrium bulk magnetization. L is chosen so that $f(1)=1/2$.] Results for quenches to T_c will be similarly affected — the dynamical exponent will be underestimated while ρ relaxes towards equilibrium [9].

A renormalized kinetic coefficient alone will not affect *scaled* correlations. However, Kawasaki exchange also allows infinite-range energy transfer through the system. For example, at $T=0$, an isolated spin (four broken bonds) may hop freely through the system by spin exchange with bulk spins (no broken bonds). Similarly, a ''bump'' on a flat interface (with one broken bond) may hop to any other flat interface of the system. Effects of this energy transport might show up at low temperatures in nonuniversal effects such as spatial anisotropy in the late stages of the quench [5]. It is unclear if nonlinear effects would change the autocorrelation results of Sire and Majumdar [4], who used this algorithm at $T=0$.

A faster and safer algorithm was proposed by Creutz [6]. The system is coupled to a small spin reservoir (here of size 2). Single spin flips accepted by normal kinetic Ising model

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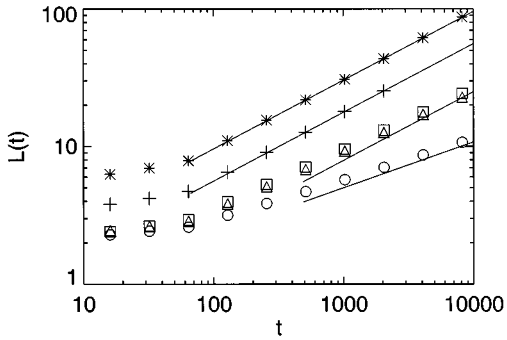

FIG. 1. Length scale $L(t)$ for nonconserved (stars), Creutz (pluses), Kawasaki $T=0.9T_c$ (triangle), and Kawasaki $T=0$ (circles). The system sizes are 2048^2, 1024^2, 512^2, and 512^2, respectively, with at least 20 samples in each system. We also show $L/\sqrt{\rho}$ for the $T=0$ Kawasaki quench (squares), which approaches $t^{1/2}$, as expected. The upper three lines show $t^{1/2}$, while the lowest line shows $t^{1/3}$.

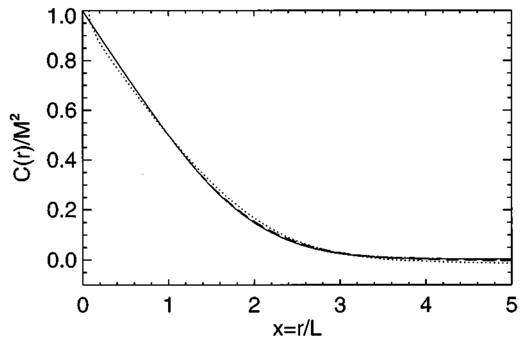

FIG. 2. Scaled correlations, divided by the equilibrium magnetization squared, from the latest times of simulations shown in the previous figure. Solid, dashed, dot-dashed, and dotted lines are nonconserved, Creutz $T=0$, Kawasaki $T=0$, and Kawasaki $T=0.9T_c$, respectively.

dynamics are subject to the additional condition that the required spin change (± 2) can be extracted from the reservoir. The dynamics of the system plus reservoir are microcanonical in the magnetization, and there are none of the questions of energy transport that we have just raised for infinite-range Kawasaki exchange [10]. As a result the RG results directly apply and a growth law of $L\sim t^{1/2}$ is indeed seen [3].

To check these arguments we simulated critical quenches, with $\langle\phi\rangle=0$, for nonconserved and also for globally conserved systems with both Creutz and Kawasaki dynamics. For off-critical quenches similar results apply. In Fig. 1 we see the asymptotic $t^{1/3}$ growth for $T=0$ Kawasaki exchange, and reconfirm $t^{1/2}$ growth for the other cases. To test the rescaling of the kinetic prefactor in the Kawasaki algorithm, we show a quench to $T=0.9T_c$ and also $L/\sqrt{\rho}$ for the quench to $T=0$. Both of these approach the expected $t^{1/2}$ growth at late times, though with a slow crossover. In Fig. 2, we see that all of the models have similar spherically averaged scaled correlations. (Anisotropies are too small to see for these critical quenches [5].) The correlations for the Kawasaki model are slightly different, however, this seems to be a transient effect. (Strong finite-size effects in the $T=0.9T_c$ quench, after the latest time shown, limit the duration of the simulation.)

In conclusion, we see that an infinite-range Kawasaki exchange implementation of global conservation laws has activated kinetics, with an anomalous $L\sim t^{1/3}$ growth at $T=0$. In addition, Kawasaki dynamics leads to long-range energy transport. The Creutz algorithm, on the other hand, is not activated and has no long-range energy transport. It provides a faster and better controlled implementation of global conservation laws, and should exhibit the expected $t^{1/2}$ growth at all temperatures.

This work was supported by EPSRC Grant No. GR/J78044.

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[9] This may be the cause of the anomalously small dynamical critical exponent seen by Tamayo and Klein [7] with infinite-range Kawasaki exchange.
[10] The Creutz algorithm must not be implemented with a sublattice update since the sweep direction generates anomalous spatial anisotropies.