Critical Dynamics, Spinodal Decomposition, and Conservation Laws

James F. Annett and Jayanth R. Banavar
Department of Physics and Materials Research Laboratory, Pennsylvania State University, 104 Davey Laboratory, University Park, Pennsylvania 16802
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A simple acceleration algorithm for Ising systems with conserved magnetization (model B) is presented. The dynamical critical exponent and the domain growth exponent in spinodal decomposition are found to be equal to those observed for model A systems with no conservation law. Our results demonstrate that systems with global conservation laws are in the same dynamical universality class as systems with no conservation laws.

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There are three principal themes in this Letter. First, a new acceleration algorithm is proposed for Ising spin systems having a conserved magnetization (model B) [1,2]. Physical arguments (for a one-dimensional system) and detailed computer simulations (in two dimensions) show that the dynamic critical exponent z (defined by the relation $\tau \sim L^z$, where τ is the correlation time and L the linear dimension of the system at criticality) for this algorithm is the same as that obtained for model A, a system with no conservation laws. Second, we have used our algorithm to study the dynamics of spinodal decomposition [3] of a 2D Ising system with conserved magnetization following the quench from a high-temperature homogeneous phase into the two-phase coexistence region. We find that in the late-time scaling regime, the exponent n characterizing the growth of the characteristic domain size R ($R \sim t^n$) is the same as that for a model A system ($n=\frac{1}{2}$) and different from the conventional model B result ($n=\frac{1}{3}$). Third, our results are consistent with recent predictions by Bray based on renormalization-group arguments [4–6]. They thus have a bearing on the recent controversy between Bray and Tamayo and Klein [7,8] (TK). We have studied one of the two versions of the TK model and find that the TK exponent is equal to the model A result, in contradiction to their 2D computer-simulation results. Our results show that global conservation laws are irrelevant in determining the dynamical universality class, as argued recently by Bray [4–6].

Our algorithm for the Ising system is a generalization of Glauber dynamics for model A—it consists of single spin flips governed by the usual Metropolis [9] rules. The global conservation of magnetization at a desired value M_0 (model B) is enforced by a Creutz "demon" or bag [10]. Spin flips are only allowed if the total sample magnetization after the spin flip, M, lies in the range $M_0-\delta \leq M \leq M_0+\delta$. Thus our algorithm smoothly extrapolates from model A (unbounded δ) to model B ($\delta=0$). In practice, all our calculations have been carried out with $M_0=0$, $\delta=2$. Our principal result is that the exponents z and n are independent of whether $\delta=2$ or δ is unbounded, and correspond to the model A results. Note that $\delta=2$ in the thermodynamic limit is a conserved magnetization system.

Dynamical critical exponent.—For $d=1$, the value of z may be obtained using random-walk arguments, once the fastest way for the motion of the domain wall has been identified. The physical arguments of Cordery, Sarker, and Tobochnik [11] are applicable in a straightforward manner to our generalized algorithm and yield $z=2=z_A$. (In both our algorithm and model A, the correlation time τ is the time for a domain wall to move a distance equal to the correlation length ξ. This random walk takes a time of order ξ^2 leading to $z=2$.)

For $d=2$, we have carried out detailed Monte Carlo simulations for a sequence of square lattices of sides 16, 24, 32, 48, 64, 96, and 128. Each lattice was sampled for 10^6 lattice updates (except for $L=128$ for which 400000 updates were used) and an ensemble of ten statistically independent lattices were considered for each size. The energy-energy correlation function $c(t)=\langle[E(t)-\langle E\rangle]\times[E(0)-\langle E\rangle]\rangle/\langle(E-\langle E\rangle)^2\rangle$ was calculated. For long enough times, the correlation function has a simple exponential decay:

$$c(t) \simeq a e^{-t/\tau} .$$

The region between when the initial transients have decayed and before the statistical noise grows too big is considered for a nonlinear fit of the above form and an extraction of τ. Typically, the data fit was carried out in the range $e^{-6} < c(t) < e^{-2.5}$. A typical fit is shown in Fig. 1. The scaling of τ with sample size L gives the dynamical critical exponent z:

$$\tau \simeq L^z .$$

Our fit (Fig. 2) gives $z=2.13\pm0.07$ and is consistent with that expected for model A [12,13].

Domain growth scaling in spinodal decomposition.—We have carried out ten independent runs on a 256×256 lattice starting from a random state with $M=0$ and quenching instantaneously to $T=0.96T_c$. The characteristic length scale of the domain R is taken to be

$$R=2\pi/\bar{k}=2\pi\int_0^\infty S(k)dk \bigg/ \int_0^\infty kS(k)dk ,$$

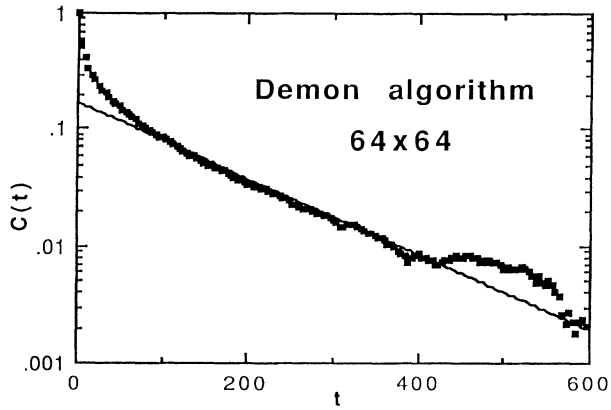

FIG. 1. Correlation function for the demon algorithm with $\delta=2$. The data are the average of ten independent runs each of 10^6 lattice updates. The line is a nonlinear fit by an exponential over the range $e^{-6} < c(t) < e^{-2.5}$.

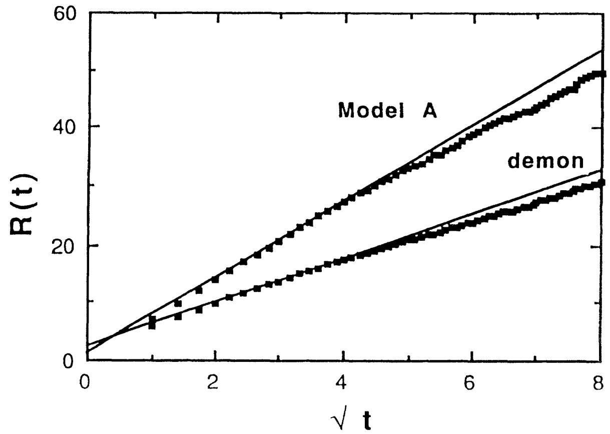

FIG. 3. Domain size $R(t)$ after quenching a 256×256 lattice to $0.96T_c$ vs $t^{1/2}$ for model A ($\delta=\infty$) and the demon algorithm ($\delta=2$).

where $S(k)$ is the spherically averaged structure factor [14]. Figure 3 shows a plot of R vs $t^{1/2}$ for both our algorithm and for model A dynamics. The deviations from a linear behavior at large t are due to finite-size effects. Both algorithms are consistent with $R \sim t^n$ with $n=\frac{1}{2}$, the accepted value for model A dynamics.

Tamayo-Klein algorithms.— We note that recently TK have proposed two algorithms for Ising systems with globally conserved magnetization. These are similar and involve simultaneous flips of pairs of spins according to either Kawasaki spin exchange [15] at arbitrary range or using a Creutz domain rather than purely single spin flips. In one dimension, for their algorithm $z=3$ and is greater than that for model A ($z=2$). Monte Carlo calculations by TK in two dimensions are suggestive of $z=2-\eta=\frac{7}{4}$. Strikingly, this value of z is lower than that expected for model A ($z_A \approx 2.18$) and thereby

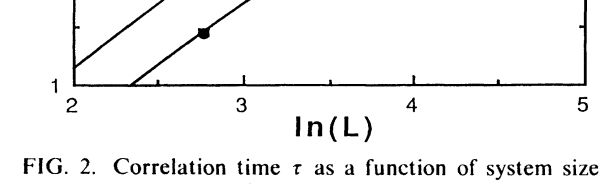

FIG. 2. Correlation time τ as a function of system size for the demon with $\delta=2$ (solid circles) and the TK algorithm (open circles).

violates the recent prediction based on renormalization-group arguments presented by Bray [$z_{TK}=\max(z_A, 2-\eta)=z_A$]. Our algorithm is a variant of the TK algorithms— unlike their case of flips of spin pairs, we attempt a single spin flip. On physical grounds, one would expect the z for our algorithm to be equal to z_{TK}, since our $z=z_A$ and we expect that $z_{TK}=z_A$. In order to verify this, we have carried out an analysis of the TK algorithm in $d=2$. Specifically, for an infinite-range Kawasaki spin-exchange algorithm, the dynamical critical exponent is found to be equal to 2.25 ± 0.12 (consistent with z_A), as shown in Fig. 2. This value is inconsistent with the earlier estimate due to TK and is in accord with the prediction of Bray.

In summary, we have presented a simple generalization of model A dynamics that extrapolates from a system with no conservation laws to one with a conserved magnetization. In the latter limiting case, our analysis has shown that both the dynamical critical exponent and the domain growth scaling exponent in spinodal decomposition are the same as in model A (even though the magnetization conservation law is enforced). Our results show that global conservation laws do *not* change the dynamical universality class. Rather, our results for the exponents are in accord with the renormalization-group arguments and bounds of Bray. Indeed, according to these bounds, our algorithm is the best that one may do within the realm of single spin flips. It remains a challenge to work out the analog of the Swendsen-Wang algorithm [16] involving flips of large clusters for systems with conserved magnetization.

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