Critical Dynamics and Global Conservation Laws

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(Received 23 June 1989)

We consider the effect on critical dynamics of global, rather than local, conservation laws. Restricting our consideration to model B (conserved order parameter) we present theoretical arguments and numerical evidence that global conservation is sufficient to establish the universality class of model B and can be used to construct faster algorithms for the calculation of dynamic critical exponents.

PACS numbers: 64.60.Fr, 05.50.+q, 64.60.Ht, 75.40.Mg

The seminal work of Hohenberg, Halperin, and Ma provides a framework within which one can understand a great deal about dynamical evolution in the neighborhood of the critical point.[1] However, with the advent of nonlocal acceleration algorithms[2-4] that eliminate or reduce critical slowing down, new questions are being raised which were not addressed in previous studies. In particular, if the new *nonlocal* acceleration algorithms are to be adapted to dynamics other than model A (e.g., Glauber dynamics) we are forced to consider whether global conservation laws are sufficient to establish dynamic universality classes or whether local conservation is essential. In this Letter we consider this question for two dynamical models that only conserve magnetization globally. These models, which are a variation of model B which we call model B', are studied numerically on the nearest-neighbor Ising model in $d=2$. We also discuss analytic results in $d=1$ and theoretical arguments in $d\geq 2$.

Consider a lattice with an Ising spin at each site. The Hamiltonian is given by

$$-\beta H = K\sum_{\langle ij\rangle} S_i S_j + h\sum_i S_i , \tag{1}$$

where $\beta = 1/k_B T$, $S_i = \pm 1$, h is the external field, and K is the ferromagnetic coupling. In order to specify a dynamics in these models we must also specify a set of conservation laws. In model A in the Hohenberg-Halperin classification[1] nothing is conserved. In model B the magnetization is conserved. The important point to note is that the conservation law is local; i.e., in order for the magnetization to change in a region specified by some boundary there must be diffusion of the magnetization across that boundary.

The equation of motion that governs the evolution of these models[1] is

$$\frac{\partial\psi(\mathbf{x},t)}{\partial t} = -\Gamma_0\frac{\delta F(\psi)}{\delta\psi} + \theta(\mathbf{x},t) + \Gamma_0 h(\mathbf{x},t) , \tag{2}$$

where

$$F(\psi) = \int dx^d \{[\nabla\psi(\mathbf{x})]^2 + \epsilon\psi^2(\mathbf{x}) + \psi^4(\mathbf{x})\} \tag{3}$$

is the Landau-Ginzburg free energy,[5] $\epsilon = (T-T_c)/T_c$, $\psi(\mathbf{x})$ is the order parameter (magnetization in Ising models), $h(\mathbf{x},t)$ is the applied field, $\theta(\mathbf{x},t)$ is a Gaussian noise with $\langle\theta\rangle = 0$, and

$$\langle\theta(\mathbf{x},t)\theta(\mathbf{x}',t')\rangle = 2\Gamma_0\delta(\mathbf{x}-\mathbf{x}')\delta(t-t') . \tag{4}$$

The parameter Γ_0 determines whether Eq. (2) describes evolution with a conserved or nonconserved order parameter.[1] For model A, Γ_0 is a constant, and for model B, $\Gamma_0 = -\lambda_0\nabla^2$. The parameter λ_0 sets the time scale.

The most frequently used algorithm to obtain model-B dynamics with Ising models is Kawasaki spin exchange[6] in which nearest-neighbor spins of opposite sign are exchanged if the energy criteria are met.[7] The interchange of nearest-neighbor pairs enforces a conservation on the order parameter which is clearly maintained on all length scales. With this method one can measure the critical exponents that characterize the slowing down of the dynamics as the critical point is approached. In particular, for model B we measure the energy autocorrelation function $\langle E(t)E(0)\rangle$ which is expected to decay as

$$\langle E(t)E(0)\rangle \sim e^{-t/\tau} \tag{5}$$

for t large. The relaxation time τ diverges as ξ^z as the critical point is approached, where ξ is the correlation length. The exponent z which characterizes critical slowing down is known, for model B, to be equal to $4-\eta$ in Ising models[1] with $d\geq 2$ and 5 in[8,9] $d=1$.

We have employed two algorithms to investigate the effect of global conservation on z. The first employs a Creutz demon[10] which has a "bag" in which it can carry magnetization. The demon visits each site at random. If a flip of one or more spins is to be performed in the neighborhood of a site, the demon bag must be checked to see if it has enough room to accommodate the flip. For example, suppose we associate spins which are down with particles and spin up with holes. We then specify, in this example, that our demon can only carry up to two particles. The algorithm then proceeds by visiting a site in the lattice at random and choosing, also at random, one of its nearest neighbors. This pair of spins is now flipped using the standard Metropolis criterion. Howev-

er, if the flip increases or decreases the number of particles the demon must be consulted to see if it can accept or give up the requisite number. If the demon constraint is satisfied the spins are flipped. If it is not, the flip is not made and the demon goes onto the next site.

Clearly this algorithm restricts the magnetization to a shell of finite width which depends on the bag size. If we allow the bag size to go to infinity we recover the Metropolis algorithm for model A. Since the demon hops randomly carrying magnetization in its bag to arbitrarily distant sites, the magnetization is not conserved locally for a nonzero bag size even in an approximate manner; i.e., the magnetization does not diffuse. With this algorithm we can study the effect of global conservation on z. Moreover, since the algorithm also contains a subset of spin flips that are identical to nearest-neighbor Kawasaki exchanges, the limit of the bag size going to zero produces the Kawasaki algorithm. Consequently, we can vary from model A to model B by varying the bag size.

The second algorithm we study is simply Kawasaki exchange of spins separated by an arbitrary distance. This algorithm will have the same z as the one described above as can be seen from the following argument. Consider a sequence of flips in the Creutz algorithm defined above that begins with a pair of spins flipped from down to up and suppose we have again set the bag size at two. This sets the demon so that no additional down-to-up flips can be made until an up-to-down flip of a pair of spins resets the demons to zero. Until the resetting, only interchanges that keep the magnetization fixed are allowed. As the magnetization per spin of the system is neither zero or one, the time between an up-to-down pair flip and a down-to-up flip is finite. With this procedure we are performing two types of updates. A finite fraction of the flips are simply *nearest-neighbor* Kawasaki spin exchange and the rest of the flips are simply up-down pairs interchanged with a finite time delay. Since the finite time delay and the fact that we are flipping four spins in pairs rather than one up-down pair will not affect the universality class, we can consider this part of our procedure as Kawasaki exchange with an arbitrary distance between the pair or pairs of spins exchanged. We can view this procedure for arbitrary bag size as having spin-interchange steps in which the interchange with the spin partner is delayed by a time set by the bag size and accomplished with an arbitrarily distant partner.

The average time to restore magnetization to the demon is a function of the size of the demon bag (which is the magnetization credit limit). In this way a time scale is introduced; below this scale the dynamics appears as model A because the effect of the conservation law is not felt. At large times, above that scale, the magnetization debt has been payed back and then the true nature of the dynamics (i.e., the conservation law) will be seen in the slowest relaxation time of the system. Before we discuss what z we should expect for the demon algorithm we discuss the Kawasaki exchange with arbitrary-distance flips.

In $d=1$ the exponent z equals 5 for nearest-neighbor Kawasaki exchange.[8,9] For Kawasaki exchange with arbitrary-distance flips the exponent[11] (z') equals 3. This can be easily derived as seen from the following argument: Since $T_c \sim 0$, the spins flipped will always be on domain walls. Each site in the lattice is visited once in a Monte Carlo update; hence the probability of obtaining a pair of spins of opposite sign on domain walls is proportional to ξ^{-1}. The domain-wall motion induces either a random walk of the domain walls in pairs, which will annihilate domains in up-down pairs, or a random walk of a single domain until it merges with one of the same sign. In either case the random walk must cover a distance ξ. Taken together these two processes lead to a relaxation time which scales as ξ^3.

In order to understand this process in higher dimensions we return to Eq. (2). The term $\Gamma_0 = -\lambda_0 \nabla^2$ sets the time scale through the parameter λ_0. If we were to change the "hopping distance" associated with the diffusion process in model B by a fixed factor l then we would multiply λ_0 by l^2. If we ignore the noise term for the moment (i.e., in the mean-field approximation) this is equivalent to rescaling time. That is t in Eq. (2) is replaced by $\tilde{t} = l^2 t$.

Including the noise term does not change the result. If we replace t and t' by $\tilde{t}$ and $\tilde{t}'$, respectively, and multiply λ_0 and $\delta(\tilde{t}-\tilde{t}')$ (to preserve normalization) by l^2, then Eq. (4) implies that $\theta(\mathbf{x},t) \rightarrow l^2 \theta(\mathbf{x},\tilde{t})$.

Since the process we are considering is the large-time limit of the approach to equilibrium, we expect no average spatial inhomogeneity. Hence, the "hopping distance" we use can be treated as a random variable. This implies that we multiply λ_0 by the average $\bar{l}^2$. We should point out that a slight bias towards longer-range flips occurs due to the ferromagnetic correlation between the spin chosen initially and its neighbors. This correlation decays with a power law at the critical point and leads to a higher-order correction which does not alter the dominant scaling behavior. For pairs chosen at random $\bar{l}^2 \sim L^2$, where L is the linear dimension of the system. From Eq. (2) and the above discussion we obtain

$$\tau \sim \xi^z / L^2 . \tag{6}$$

In order to test this result numerically we performed Monte Carlo simulations for model B with arbitrary-distance flips on Ising models in $d=2$. To obtain values for z we used finite-size scaling which fixes $L=\xi$. From Eq. (6) then we have $z'=z-2$ which is consistent with the one-dimensional result.

In Fig. 1 we present the data for τ in a log-log plot. The slope of the line is z'. The best fit to the data gives $z' = 1.78 \pm 0.04$, consistent with our analysis.

Returning to the demon algorithm, we expect that the result embodied in Eq. (6) will still apply. This follows

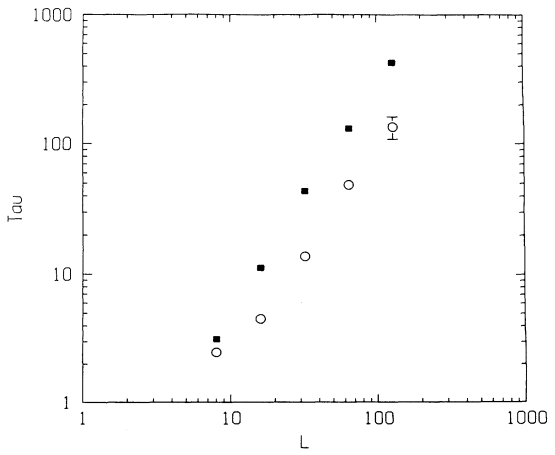

FIG. 1. Log-log plot of the energy autocorrelation time vs lattice size for 2D Ising-Kawasaki dynamics with arbitrary-distance spin exchange (squares) and nonlocal demon (circles). The critical exponent z' equals 1.78 ± 0.04 for the arbitrary-distance Kawasaki and 1.74 ± 0.11 for the demon algorithm. These results are consistent with $z' = z - 2$. Each point represents at least 500000 trials and the width of the points is greater than the statistical error unless otherwise specified.

from the decomposition of this algorithm into a nearest-neighbor Kawasaki exchange and a Kawasaki exchange with arbitrary-distance flips as discussed above. Since $z' < z$, it follows that the decorrelation will be dominated by the arbitrary-range Kawasaki exchange which is the faster of the two algorithms.

In the figure we also present the data for τ in a log-log plot obtained with the demon algorithm. The best fit for z' is 1.74 ± 0.11, again consistent with our arguments.

It is somewhat surprising at first that a spin-exchange algorithm, even one with arbitrary distance between exchanged spins, has a lower value of z than a spin-flip algorithm. One way to understand this is to realize that the approach to equilibrium is determined by two factors: the size of the region of phase space that the system must sample in order to find that part corresponding to the equilibrium state and the speed at which phase space is sampled. By changing the algorithm from a local diffusive evolution to one of hopping with arbitrary distance we have sped up the sampling of phase space. We have no proof but it seems reasonable to assume that the arbitrary-distance hopping algorithm samples phase space as fast as a spin-flip algorithm. Moreover, by keeping the global magnetization constraint we have restricted the region of phase space the system must sample in order to find equilibrium. For these reasons we expect the nonlocal exchange algorithm to be faster than the spin flip.

In conclusion, we have argued that global conservation of the order parameter is sufficient to establish the universality class of model B with a rather trivial modification to the exponent z. The demon form of the algorithm is easily generalized to other conservation laws. This has significant implications for the adaptation of nonlocal acceleration algorithms to systems with conservation laws and the use of these algorithms to obtain information about dynamics. Clearly we have not presented a proof; however, the heuristic arguments and the numerical data are, we believe, quite convincing. Moreover, we would hope that this work would stimulate work of a more rigorous nature. In addition, the simple modification of $z' = z - 2$ when finite-size scaling is used makes the nonlocal algorithm, with either arbitrary-distance spin exchange, or the more general demon method, a valuable tool for obtaining accurate values for z in dynamical models with conservation laws.

We would like to acknowledge many useful conversations with T. Ray, M. Creutz, H. Gould, A. Ferrenberg, R. Edwards, R. Swendsen, A. Sokal, N. Jan, J. Tobochnik, R. Brower, and D. Forster. This project was supported in part by a grant from the Office of Naval Research. We also wish to acknowledge the support of the Academic Computing Center at Boston University.

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