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Kawasaki Dynamics with Infinite-Range Spin Exchange

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The essential feature of the Kawasaki model is the conserved order parameter, which places the model in class B of the Halperin, Hoheberg, and Ma classification. We have studied the energy relaxation of this model in one and two dimensions with the added feature that spin exchange may take place between any pair of sites within the system. Our results for the dynamic exponent z are indistinguishable from those for class A models, in which the order parameter is not conserved.

KEY WORDS: Dynamic critical exponents; Glauber and Kawasaki dynamics; Ising model; Monte Carlo renormalization.

1. INTRODUCTION

Halperin *et al.*[1] and Hohenberg and Halperin[2] proposed a classification for thermodynamic systems near the critical temperature which suggests that the dynamical critical exponents depend on the conservation laws. In particular, the Ising model with Glauber dynamics in which neither the order parameter (magnetization) nor the energy is conserved lies in class A ($z = 2 + c\eta$, where c is a constant of order unity), while the same model but with Kawasaki dynamics (nearest-neighbor spin exchange), in which the magnetization is conserved, falls into class B ($z = 4 - \eta$). In this paper, we consider the effect of allowing spin exchange between any pair of sites within the system while maintaining global conservation of the magnetization, with a view to testing the role played by global versus local conservation laws.

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In recent work[3] we considered the Ising Hamiltonian

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j \tag{1}$$

where $\langle ij \rangle$ are the nearest neighbor pairs and σ_i are the usual Ising spin variables ± 1. We then allowed spin exchange within a local region (larger than nearest-neighbor but much less than the size of the system) without alteration of the Hamiltonian. This resulted in a simple rescaling of time so that the relaxation appeared faster than for the usual Kawasaki dynamics. The dynamic exponent was, however, exactly the same, because length rescaling maps all models with finite spin exchange range back onto the nearest-neighbor Kawasaki fixed point. This is obviously not so when the spin exchange range is infinite (i.e., of the order of the size of the system) and it is interesting to investigate whether this case flows to the same or to another distinct fixed point. The recent work of Tamayo and Klein[4,5] also considered this problem. They concluded that this model belongs to a new universality class, distinct from both the Glauber (class A) and the Kawasaki (class B) dynamic fixed points. In fact, their result is consistent with the value $z = 2 - \eta$, which arises from the simple analysis of rescaling the characteristic time τ by a factor ξ^2, where ξ is the correlation length. Thus, they find

$$\tau \sim \frac{\xi^z}{\xi^2} \sim \xi^{2-\eta}$$

for a system with conserved magnetization but long-range spin exchange. This result is surprising since it suggests that double spin flips *with global conservation* lead to faster relaxation than the single spin flips of Glauber dynamics, *which has fewer constraints!*

2. MONTE CARLO RENORMALIZATION GROUP

The method used here for determining the dynamic critical exponent in two dimensions was introduced by Jan *et al.*[16] and the theory was developed further by Stauffer[7] and others.[8–10] We consider, via Monte Carlo simulation, relaxation of the appropriate thermodynamic quantity and of renormalized images embedded in the original Monte Carlo configurations. For example, at the critical temperature, we renormalize the original system into cells of size b. The magnetization of the renormalized system is then given by $M_b = g(t/b^z)$, where g is a scaling function. Comparing two such renormalized systems at the time when $M_{b1} = M_{b2}$,

we find $(t_1/b_1^z) = (t_2/b_2^z)$. This technique is very convenient and is considerably less demanding of computer time than most alternatives.

3. RESULTS

3.1. $d = 1$

In one dimension we simulate Ising chains of between 20,000 and 50,000 spins set initially up or down at random.

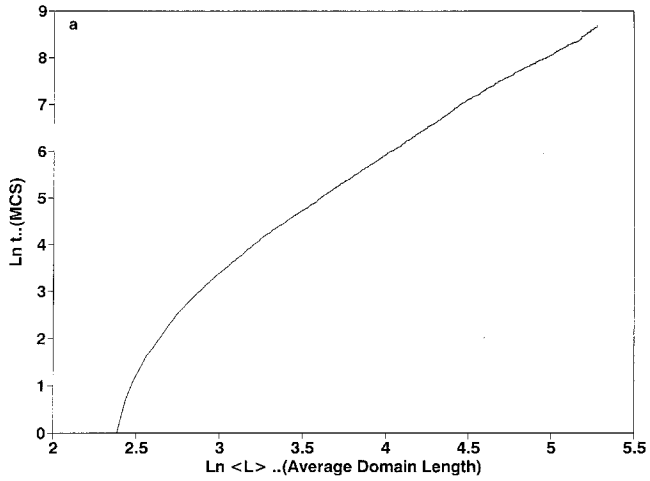
At $T = T_c$ ($\equiv 0$), where it is energetically impossible to form a domain of length one, i.e., a single spin within a cluster of spins of the opposite sign, exchange was allowed only between spins at domain walls. We find $z = 2.00 \pm 0.02$, compatible with ref. 4. As expected, this result is independent of whether the exchange took place between neighboring domain walls or *any* two domain walls (Fig. 1a).

At just above the critical temperature $T = T_c^+$ ($\equiv 0^+$) the time taken for domains to merge will be very much longer than the diffusion time for a single-spin domain.[11] Consequently, at the start and after each Monte Carlo Step, all such single-spin domains were allowed to diffuse to a boundary as soon as they were created. This meant that only the domain boundaries had to be stored, since exchange involving spins anywhere else would necessarily create single-spin domains. It is here that our arguments diverge somewhat from those of Tamayo and Klein.[4,5] There are two important variants to be considered: (i) nearest-neighbor exchange and (ii) exchange between any two spins of opposite orientation. We find that, as in ref. 11, case (i) leads to a dynamic exponent $z = 3$ (Fig. 1b), while (ii) is identical to the case at $T = 0$, and $z = 2$.

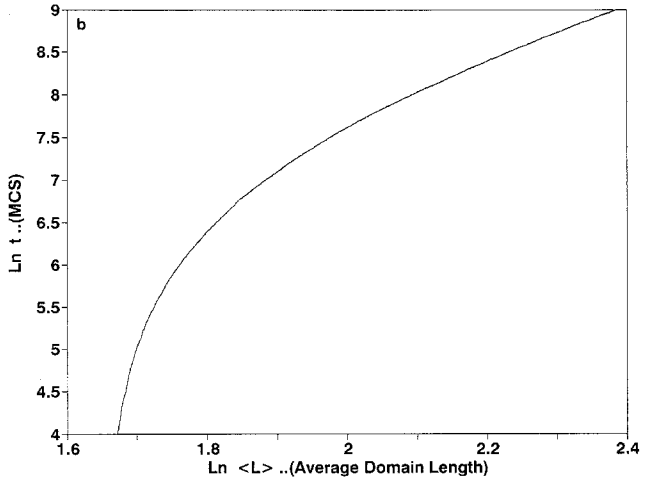
The difference between the result $z = 3$ and the value $z = 5$ given by Cordery *et al.*[13] and Zwerger[14] for the nearest-neighbor exchange is also explained by the temperature not being exactly T_c.

3.2. $d = 2$

In two dimensions we considered the Ising model at $T = T_c$ with magnetization equal to zero. The usual Kawasaki procedure was implemented, but with the modification that the spin exchange might occur with equal probability between any two sites of the system. The Hamiltonian is still defined by Eq. (1). The system was initialized in a random state (~ 0 energy) and then allowed to evolve toward equilibrium. The relaxation curve and the curves for the renormalized images are shown in Fig. 2. We obtain $z = 2.23 \pm 0.05$, which is not consistent with the numerical results $z' = 1.78 \pm 0.04$ and $z' = 1.74 \pm 0.11$ quoted in Ref. 4.



(a)



(b)

Fig. 1. (a) Relaxation curve for the one-dimensional Kawasaki model with exchange allowed between spins at any domain boundaries. The asymptotic slope determines the dynamic exponent z, which is 2.00 ± 0.02. (b) Relaxation curve for the one-dimensional Kawasaki model with exchange allowed between spins at neighboring domain boundaries. The domain length is L and the probability of exchange is $1/L$. The asymptotic slope determines the dynamic exponent z, which is 3.1 ± 0.1.

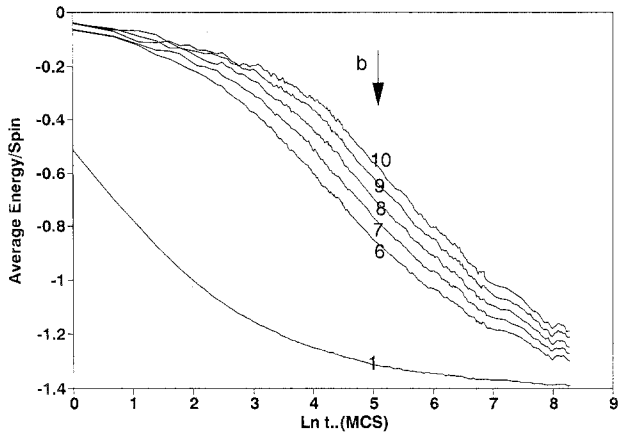


Fig. 2. Relaxation curves for the 2D Kawasaki model with exchange allowed between any pair of spins in the system. The system comprises 10^6 spins and was averaged over ten runs. The dynamic exponent is obtained by constructing a replica on semitransparent paper and shifting along the time axis until the curves for different values of b coincide. Calculation of $\ln(t/t')/\ln(b/b')$ then leads to a value $z = 2.23 \pm 0.06$.

4. CONCLUSION

The replacement of the constraint of local conservation of the magnetization by a global constraint leads to dynamical properties which are distinct from those observed for the nearest-neighbor Kawasaki model. The results we have found differ from those reported in ref. 4, where the authors considered the relaxation of the total system at equilibrium. Our approach, however, is slightly different, in that we consider the behavior of renormalized cells which are much smaller than either the length of the system or the range of the spin exchange. It is not expected that these cells will have a larger dynamic exponent than that measured for the total system.

A recent paper by Bray[12] argues that the analysis of ref. 4 cannot be extended to a range in which the dynamical exponent of model B would be less than that of model A. Our results for $d = 2$ are compatible with this statement and with $z = 2 + c\eta$ with $c \approx 0.7261$,[1] the dynamic exponent of the 2D Ising model with Glauber dynamics. We find the dynamic exponent for our model to be indistinguishable from that measured for model A with nonconserved order parameter!

The case for $d = 1$ is somewhat ambiguous; the results depend on which version of the model is considered. This is strictly because in one dimension the critical temperature is zero. The version which is closest in

spirit to the 2D situation, i.e., the exchange between any pair of oppositely oriented spins in the lattice, leads to $z = 2$, the same value as for the non-conserved model A.

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