

Dynamic Monte Carlo Renormalization Group. II

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The dynamic Monte Carlo Renormalization group method introduced by Jan, Moseley, and Stauffer is used to determine the dynamic exponent of the Ising model with conserved magnetization in two dimensions. We present an explicit theoretical basis for the method and expand on the original results for the Kawasaki model. The new result clearly demonstrates the validity of the method and the value of the dynamic exponent, $z = 3.79 \pm 0.05$, supports the conclusion of Halperin, Hohenberg, and Ma.

KEY WORDS: Monte Carlo; renormalization group; dynamic exponent; Kawasaki model.

1. INTRODUCTION

The history of the combination of renormalization group (RG) and Monte Carlo simulation was outlined by Jan *et al.* (JMS).⁽¹⁾ They also introduced a new dynamical RG which compares favorably in its computational simplicity with the large-cell RG of Reynolds *et al.*,⁽³⁾ used for calculating static exponents. Reasonable results were obtained with a very significant reduction of computing effort and the method has been subsequently applied to the Potts and the eight-vertex models.⁽⁴⁾ In Section 2 we review the theoretical foundations in sufficient detail to illustrate the distinction between this RG and conventional, finite-size scaling.

The size of the systems analyzed to determine z for the Glauber model (magnetization not conserved) has been increased from $\sim 2 \times 10^6$ to $\sim 10^8$ spins by the use of supercomputers⁽⁵⁾ and special-purpose machines.⁽⁶⁾ The Kawasaki model (conserved magnetization) has not, however, received the

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same level of attention, largely because of the greater computational effort required to reach equilibrium when compared with the Glauber model. Nevertheless, this model is of considerable interest because of its relationship to other problems, such as domain growth and order-disorder transitions.⁽⁷⁾ Our results for the Kawasaki model are presented in Section 3.

2. THEORY

2.1. Finite-Size Scaling

For a system of linear dimension L , the equilibrium magnetization obeys the finite scaling ansatz⁽⁸⁾

$$M_L(T, t = \infty) = L^{-\beta/\nu} f[(T - T_c)L^{1/\nu}] \quad (1)$$

This form is well known and was reviewed in ref. 9.

For the nonequilibrium situation, starting with all spins up, the system relaxes to equilibrium as

$$M_L(t) = L^{-\beta/\nu} \tilde{f}[(T - T_c)L^{1/\nu}, t/L^z] \quad (2)$$

At the critical temperature this reduces to

$$M_L(t) = L^{-\beta/\nu} g(t/L^z) \quad (3)$$

Now, by comparing times t_1 and t_2 at which $[M_1/L_1^{-\beta/\nu}]$ is equal to $[M_2/L_2^{-\beta/\nu}]$, we find

$$t_1/L_1^z = t_2/L_2^z$$

or, for $M_1 = M_2$,

$$t_1/L_1^{z + \beta/\nu} = t_2/L_2^{z + \beta/\nu} \quad (4)$$

If in our simulation we calculate M_L for different values of L as a function of T , then we expect the behavior shown in Fig. 1a, with the sharp fall of M_L to zero occurring only for the infinite system.

2.2. Renormalized Scaling

Consider a Monte Carlo configuration and its renormalized images, i.e., the set of systems formed by blocking the configuration into cells and replacing the cells with renormalized spins whose states are determined by the majority of spins in that cell (see ref. 10 for a general review). The

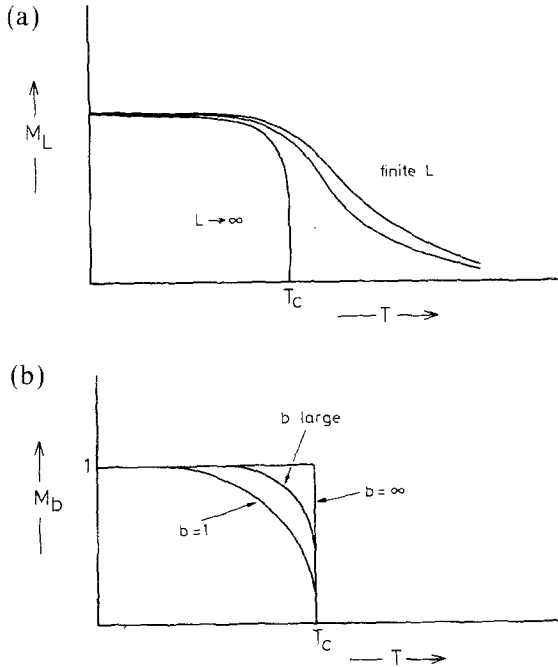


Fig. 1. (a) The magnetization M_L of a system of L^2 spins as a function of the temperature T ; T_c is the critical temperature. (b) The magnetization M_b of a system of $(L/b)^2$ superspins as a function of the temperature T .

renormalized spin replacing each cell is thus determined by the sign of the magnetization of that cell. Thus, as $b \rightarrow \infty$, for T slightly below T_c one finds $|M_b| = 1$, while for $T > T_c$, $M_b = 0$, where M_b is the magnetization of the renormalized configuration whose cells are of size b .

This behavior is illustrated in Fig. 1b. Note that this is quite different from Fig. 1a and is closer to the large-cell real-space RG of Reynolds *et al.*⁽³⁾ Stauffer⁽¹¹⁾ has shown that for $L \gg b$ the finite-size scaling ansatz for the equilibrium state is

$$M_b = f[(T - T_c)b^{1/\nu}] \tag{5}$$

and the nonequilibrium situation would be described by

$$M_b = \tilde{f}[(T - T_c)b^{1/\nu}, (t/b^z)] \tag{6}$$

At the critical temperature this reduces to

$$M_b = g(t/b^z) \tag{7}$$

and there for $M_{b_1} = M_{b_2}$ we have the simple relation

$$t_1/b_1^z = t_2/b_2^z \quad (8)$$

Note that there are no factors of $L^{-\beta/\nu}$ in Eq. (6) and (8). The problem is thus reduced to the accurate determination of the times t_1 and t_2 at which the magnetizations M_{b_1} and M_{b_2} of two renormalized systems are equal.

3. RESULTS

In Fig. 2 we show the results of our simulation of the relaxation of a two-dimensional system of 600×600 spins via Kawasaki dynamics. Following JMS, we have included further neighbors in the exchange process. On this occasion, however, we have *demonstrated* that the so-called "generalized Kawasaki model" lies in the same universality class as the usual Kawasaki model, by showing that the curves for the further-neighbor exchange may be brought into coincidence with that for the nearest-neighbor exchange only, if we simply rescale the time by the relative

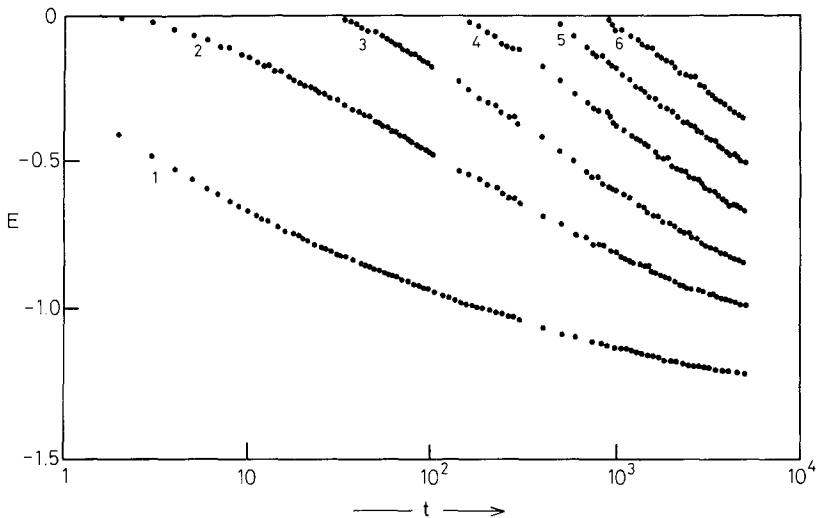


Fig. 2. Relaxation of the original energy and of the renormalized energies with time, i.e., with the number of Monte Carlo steps per spin in the original system of 600×600 spins. These curves are assembled by scaling the time axes of similar (original) systems by the ratio of the number of spins between which exchange is allowed during relaxation. The curves may then be made to coincide by shifts to the right or left along the time axis. The numbers on the data sets give b , the length rescaling factor.

Table I.
Exponent Estimates for the Two-Dimensional z :
Generalized Kawasaki Model to $t = 2 \times 10^5$ MCS

| b' | z | | | | |
|------|-------|-------|-------|-------|-------|
| | $b=8$ | $b=7$ | $b=6$ | $b=5$ | $b=4$ |
| 7 | 3.75 | | | | |
| 6 | 3.79 | 3.83 | | | |
| 5 | 3.80 | 3.86 | 3.79 | | |
| 4 | | 3.86 | 3.72 | 3.76 | |
| 3 | | | | 3.78 | 3.75 |

number of spins in the “exchange cells.” This is shown clearly in Fig. 2, which is derived from separate 600×600 systems involving 1st-, 5th-, 9th-, 14th-, and 19th-neighbor exchange. The corresponding exchange cells have 5, 25, 49, 81, and 221 spins and therefore time scaling factors of 1, 5, 9.8, 16.2, and 24.2, respectively. This scaling allows us to follow the relaxation to very much longer (effective) times than we could otherwise have achieved. The simulation was carried out on an IBM PS/2 micro-computer⁽¹²⁾ with occasional confirmatory runs on DEC Vax 11/750 and an IBM 370/168.

The results of our estimation of the exponent z are shown in Table I,

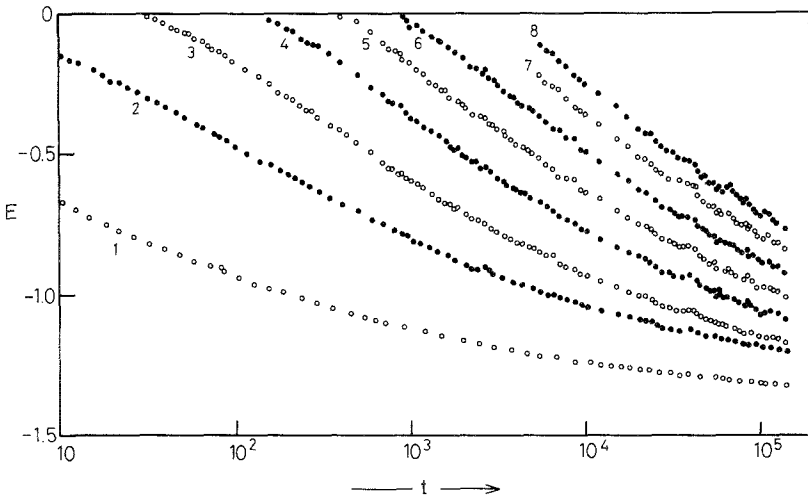


Fig. 3. Relaxation curves for the Kawasaki model. In this case exchange is only allowed between nearest neighbors and computing constraints restrict us to times too short to obtain “good” values of z .

Table II.
Exponent Estimates for the Two-Dimensional z :
Kawasaki Model to $t = 5 \times 10^3$ MCS

| b' | z | | | |
|------|---------|---------|---------|---------|
| | $b = 6$ | $b = 5$ | $b = 4$ | $b = 3$ |
| 5 | 4.26 | | | |
| 4 | 4.16 | 4.11 | | |
| 3 | 4.18 | 4.15 | 4.19 | |
| 2 | 4.19 | 4.03 | 3.76 | 3.23 |

and we conclude that $z \approx 3.79$, with a statistical error of about 0.05. Cells of size $b \times b$ and of size $b' \times b'$ are renormalized into one superspin each and the systems thus formed are compared. The exponent z is then calculated as $\ln(t_b/t_{b'})/\ln(b/b')$, where the time is obtained from the shift along the time axis of the curves for different b and b' values shown in Fig. 2 to bring them into coincidence, thereby achieving the required comparison of E_b and $E_{b'}$ over a wide time range. E_b and $E_{b'}$ are respective energies of the renormalized system b and b' . As discussed in JMS, this method is expected to give more reliable results for higher values of b and smaller ratios b/b' . The latter condition arises because the shifting necessary to bring the curve, for example, for $b = 8$ into coincidence with that for $b = 4$ requires reliance on times $< \sim 10^4$ MCS. The matching is usually more consistent when longer time regions on both curves are used (which also means greater regions of overlap). Furthermore, use of the shorter time regions will be less accurate, since the rescaling of the “generalized Kawasaki model” back to the usual, nearest-neighbor-exchange-only model cannot be accurate at short times.

In Fig. 3, we show the corresponding curves for the usual Kawasaki model without enhanced diffusion. The estimates of z are shown in Table II, and lead to $z = 4.0 \pm 0.3$. Computing constraints limit us to $\sim 5 \times 10^3$ MCS in this case—in comparison with effectively $\sim 2 \times 10^5$ MCS when we use the generalized model.

4. CONCLUSION

Our result $z = 3.79 \pm 0.05$ agrees very well with the result predicted by the Halperin *et al.*⁽²⁾ relation

$$z = 4 - \eta = 3.75$$

Comparison of this result with the earlier value $z = 3.9 \pm 0.1$ found by JMS for a 300×300 spin system confirms the effectiveness of our procedures in reducing errors due to finite-size effects as well as reducing computing effort.

We have justified the premise of this simple RG method, i.e., Eq. (7), and shown how this renormalization group is different from finite-size scaling.

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