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Monte Carlo renormalization-group studies of kinetic Ising models

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The dynamic Monte Carlo renormalization group is applied to the two-dimensional Kawasaki and three-dimensional Glauber models. Our best "matching" results for the Kawasaki model yield a value of $z = 3.80$ for the dynamical exponent, as compared with the exact value $z = 3.75$. This provides strong confirmation for the validity of this method. The results for the Glauber model are less accurate, but our estimate of $z \simeq 2.08$ is in reasonable agreement with the ϵ expansion.

The Monte Carlo renormalization group (MCRG) was originally introduced by Ma[1] for the study of the static and dynamical properties of the kinetic Ising model. A somewhat different, improved version of this MCRG was then developed by Swendsen[2] and subsequently Wilson[3] and applied to a variety of static problems in critical phenomena. Quite recently this method has been applied to the two-dimensional Glauber model[4] (with nonconserved order parameter) by Tobochnik, Sarker, and Cordery[5] to compute the dynamical exponent z. At the moment there is considerable controversy[6,7] about the validity of the various real-space dynamical renormalization groups that have been developed,[8–12] including the MCRG. In view of the importance of developing a valid real-space theory for critical dynamics and because the MCRG seems to offer the possibility of a systematic theory, we have therefore applied the procedure of Tobochnik *et al.*[5] to the two-dimensional Kawasaki model[13] (with a conserved order parameter) for which the exact value of z is thought to be[14,15] $z = 4 - \eta = 3.75$, where η is the standard correlation function exponent. As we see below, our results are in excellent agreement with this value, thus providing a strong confirmation of the validity of the dynamical MCRG. In addition, we have also considered the three-dimensional Glauber model, for which ϵ-expansion results[15,16] exist for the analogous time-dependent Ginzburg-Landau model (where $\epsilon = 4 - d$ and d is the dimensionality). Our present estimate of $z \simeq 2.08$ is in reasonable agreement with the ϵ-expansion value of $z \simeq 1.99$, but more accurate statistics will be necessary for a convincing MCRG determination, as we discuss later.

Following Tobochnik *et al.*[5] we use standard Monte Carlo methods to compute time correlation functions for an original lattice of N spins and its sequence of renormalized lattices generated by m blockings ($m = 1, 2, \ldots$). The block-spin configurations (with block spins $\{S_i^{(m)}\}$) are generated from the original spin configurations (with site spins $\{S_i\}$) by the majority rule transformation. "Ties" are broken by randomly assigning the block spins the value ± 1. It should be noted that for the Kawasaki model this procedure can occasionally violate the conservation of magnetization on the renormalized lattices, but we have found this to be a negligible effect (e.g., the average magnetization per spin is never larger than 10^{-3} for the lattices used as compared with the exact value of zero). This same renormalization procedure is also carried out for a second initial lattice of Nb^d spins, where b is the length rescaling parameter, $b = 2$. One then attempts to find two temperatures T_1 and T_2 and two times t and t' (which are related by the dynamic exponent z via $t' = tb^z$) such that correlation functions for the two different sets of lattices "match." This then determines z. Specifically, we obtain estimates of z from the conditions

$$C\{N,m,T_1;t\} = C\{Nb^d,m+1,T_2;t'\} \qquad (1)$$

and

$$E\{N,m,T_1;t\} = E\{Nb^d,m+1,T_2;t'\} \ , \qquad (2)$$

where the two correlation functions are defined as

$$C\{N,m,T;t\} \equiv \frac{1}{N^{(m)}}\left\langle \sum_i S_i^{(m)}(t) S_i^{(m)}(0) \right\rangle_{T,N} \qquad (3)$$

and

$$E\{N,m,T;t\} \equiv \frac{1}{N^{(m)}}\left\langle \sum_{\langle ij\rangle} S_i^{(m)}(t) S_j^{(m)}(0) \right\rangle_{T,N} \ . \qquad (4)$$

The sum in (4) is over nearest-neighbor pairs on a d-dimensional hypercube. The reduced Ising Hamiltonian is $H = T^{-1} \sum_{\langle ij\rangle} S_i S_j$, where T is the dimensionless temperature. The conditions (1) and (2) provide two different estimates of z which in principle one would expect to be the same but in practice will be somewhat different. We have found that our data for $E(t)$ [and to a lesser extent $C(t)$] are very well represented for sufficiently large times by the dominant exponential decay,

$$E\{N,m,T;t\} \simeq A_m^{(N)} e^{-t/\tau_m} \quad , \tag{5}$$

where τ_m is the time constant. This form has allowed us to make an estimate of the error in our matching, since (2) and (5) imply that $A_m^{(N)} = A_{m+1}^{(Nb^d)}$. We should note that since we are searching for a critical fixed point we must have $T_1 = T_2 = T_c$. We have used the exact value of the critical temperature (for the infinite system) in two dimensions and the high-temperature-series estimate in three dimensions.

Our analysis has been carried out for hypercubes of edge size eight and sixteen in both two and three dimensions, using periodic boundary conditions. A standard transition probability, w, for exchanging a pair of randomly chosen spins (Kawasaki model) or flipping a randomly chosen spin (Glauber model) was used, of the form $w = 1$ if $\Delta H < 0$ and $w = \exp(-\beta\Delta H)$ if $\Delta H \geqslant 0$. ΔH is the change in the energy resulting from the transition, and β is the inverse temperature times the Boltzmann constant.

Our results for the Kawasaki model are shown in Table I and are based on using 2.3×10^6 and 2.04×10^6 MCS (Monte Carlo steps) in computing the correlation functions for the 8×8 and 16×16 lattices, respectively. We have found that the matching conditions (3) and (4) are best satisfied for the renormalized 4×4 lattice. The results for $E(t)$ are particularly good, with the exponential decay (5) being an excellent representation of the data, as shown in Fig. 1. This matching yields as an estimate $z = 3.80$. One measure of the error in matching, given (5), is the difference between the amplitude A_m for the two 4×4 lattices. This can be obtained by extrapolating the linear fits in Fig. 1 to $t = 0$. One finds that the relative difference in the amplitudes is only 2%, so that the matching is very good. The autocorrelation function $C(t)$ is also well represented by an exponential decay if one excludes times less than $t = 40$ and 600 for the initial lattices of 8×8 and 16×16 spins, respectively, as shown in Fig. 2. The matching condition (3) is not quite as well satisfied as (4), as reflected, for example, in a relative difference of the amplitudes of the renormalized autocorrelation functions of about 5%. The resulting estimate for z is $z = 3.88$. Overall the best MCRG results are given by the analysis of $E(t)$, and we therefore consider $z = 3.80$ to be the most reliable estimate of the critical exponent. We consider the results for $E(t)$ as given in Fig. 1 to be an excellent indication of the validity of the MCRG in critical dynamics. Nevertheless, we should add two qualifications. The first is that significant finite-size effects are seen in our study, although they do not influence the determination of z. A simple manifestation of this is seen in our estimates of the equilibrium energy per spin, where we obtain 0.58 for the $N = 256$ lattice as compared with the exact result for the infinite system of $\sqrt{2}/2 \simeq 0.707$. The second finite-size effect is more subtle and results from the conservation law. This leads to block configurations for the 2×2 lattice, which are of antiferromagnetic-like nature and hence to slightly negative values of $E(t)$, as shown in Table I. This is one reason we do not use the 2×2 lattice for our matching, although a good matching occurs for $C(t)$. This effect does not arise in the Glauber model.

Finally, we note that we have carried out the same

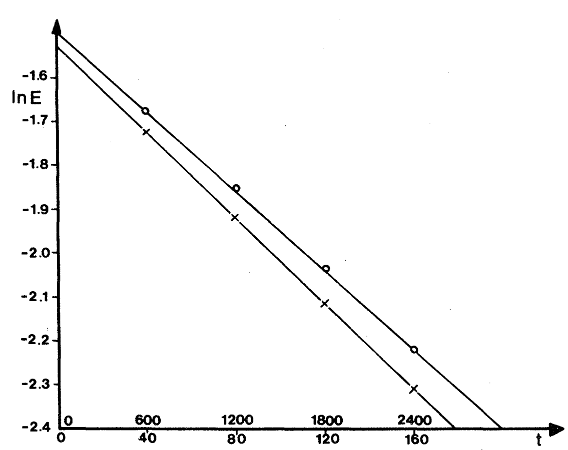

FIG. 1. Plot of $\ln E(t)$ vs t for a renormalized lattice of 4×4 spins. The data for initial lattices of 8×8 and 16×16 spins are denoted by dots and crosses, respectively.

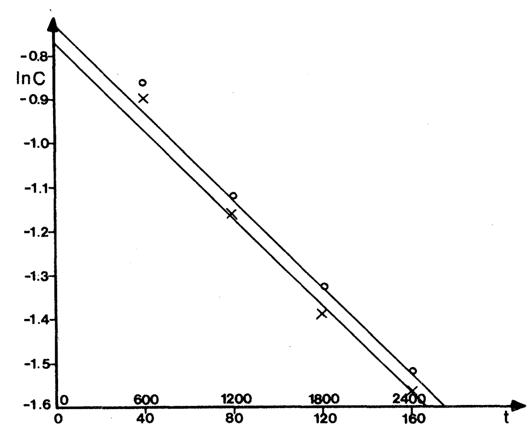

FIG. 2. Plot of $\ln C(t)$ vs t for the same systems as in Fig. 1.

TABLE I. The dynamic MCRG data for the two-dimensional Kawasaki model for the two correlation functions $E(t)$ and $C(t)$ defined in the text. The quantities N, m, and t denote the number of spins on the lattice, the number of blockings, and the time in Monte Carlo steps, respectively.

	$2^m N$	$=256$	$2^m N$	$=64$
$E(t=0)$	1	0.5799		
	2	0.4306	1	0.4555
	4	0.1894	2	0.1913
	8	−0.0396	4	−0.0584
$C(t)$		$t=600$		$t=40$
	1	0.2972		
	2	0.3473	1	0.3824
	4	0.4076	2	0.4229
	8	−0.3509	4	0.3727
$E(t)$		$t=600$		$t=40$
	1	0.2843		
	2	0.2863	1	0.3137
	4	0.1782	2	0.1871
	8	−0.0129	4	−0.0150
$C(t)$		$t=1200$		$t=80$
	1	0.2224		
	2	0.2604	1	0.2893
	4	0.3118	2	0.3264
	8	0.3016	4	0.2976
$E(t)$		$t=1200$		$t=80$
	1	0.2134		
	2	0.2201	1	0.2436
	4	0.1467	2	0.1565
	8	−0.0057	4	−0.0053
$C(t)$		$t=1800$		$t=120$
	1	0.1762		
	2	0.2053	1	0.2330
	4	0.2500	2	0.2641
	8	0.2404	4	0.2463
$E(t)$		$t=1800$		$t=120$
	1	0.1696		
	2	0.1763	1	0.1979
	4	0.1209	2	0.1306
	8	−0.0055	4	−0.0008
$C(t)$		$t=2400$		$t=160$
	1	0.1445		
	2	0.1701	1	0.1917
	4	0.2076	2	0.2188
	8	0.1876	4	0.2029
$E(t)$		$t=2400$		$t=160$
	1	0.1393		
	2	0.1450	1	0.1633
	4	0.0994	2	0.1087
	8	−0.0017	4	−0.0014

analysis for $C(t)$ and $E(t)$ for the $d=3$ Glauber model. Although we obtain results similar to that shown in Figs. 1 and 2, the matching conditions (3) and (4) are not as well satisfied as in the two-dimensional model. The relative differences in the amplitudes of the renormalized $E(t)$ and $C(t)$ for the $4\times4\times4$ lattices are, for example, about 5% and 7%, respectively. The estimate of the exponent obtained from matching $E(t)$ is $z\simeq 2.08$, which is in reasonable agreement with the ϵ-expansion estimate $z\simeq 1.99$. Nevertheless, although we have expended comparable computer time on the Kawasaki and Glauber models, we have less confidence in our estimate of the Glauber exponent. This is because we have poorer statistics in the three-dimensional case, where we have computed correlation functions using 1.15×10^5 and 7.37×10^4 MCS for the $8\times8\times8$ and $16\times16\times16$ lattices, respectively. The increase in the total number of spins involved in going from $d=2$ to 3 makes the problem of obtaining good statistics more difficult in three dimensions than in two dimensions. Nevertheless, there seems to be no difficulty in principle in obtaining an accurate estimate of z for the $d=3$ Glauber model by this method. We are in the process of doing more extensive simulation studies of this problem. In conclusion, we note that the dynamic MCRG seems to be a promising new technique. However, its successful application will require very good statistics and quite accurate matching to obtain precise exponents. As well, the ambiguity associated with determining z when one does not have an exact matching needs to be resolved. Finally, it should be noted that one advantage of this Monte Carlo method is that it avoids the difficulties associated with a direct calculation of the kinetic coefficient.[7] In this sense it seems as powerful a tool for the Glauber model as for the Kawasaki model, even though the kinetic coefficient vanishes in the former case.

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