Journal of Statistical Physics, Vol. 33, No. 1, 1983

Dynamic Monte Carlo Renormalization Group

Naeem Jan,[1,2] L. Leo Moseley,[1,3] and Dietrich Stauffer[1,4]

Received March 15, 1983

A new and simple method of applying the idea of real space renormalization group theory to the analysis of Monte Carlo configurations is proposed and applied to the Glauber kinetic Ising model in two and three dimensions, and to the Kawasaki model in two dimensions. Our method, if correct, utilizes how the system approaches its equilibrium; in contrast to most other Monte Carlo investigations there is no need to wait until equilibrium is established. The renormalization analysis takes only a small fraction of the computer time needed to produce the Monte Carlo configurations, and the results are obtained as the system relaxes at $T = T_c$, the critical temperature. The values obtained for the dynamical critical exponent, z, are 2.12 ($d = 2$) and 2.11 ($d = 3$) for the Glauber model, the 3.90 for the two-dimensional Kawasaki model. These results are in good agreement with those obtained by other methods but with smaller error bars in three dimensions.

KEY WORDS: Renormalization group; Monte Carlo; dynamic critical phenomena; Glauber and Kawasaki models; Ising model; finite-size scaling.

1. INTRODUCTION

The combination of renormalization group and Monte Carlo simulation was initiated by Ma,[1] who in a prototype analysis was able to calculate static as well as dynamic critical exponents for the two-dimensional Ising

[1] Center for Polymer Studies, Boston University, Boston, Massachusetts 02215.

[2] Permanent address: Physics Department, St. Francis Xavier University, Antigonish, Nova Scotia B2G 1C0 Canada.

[3] Permanent address: Physics Department, University of the West Indies, Cave Hill, Barbados.

[4] Permanent address: Institut für Theoretische Physik, Universität, 5000 Köln 41, West Germany.

0022-4715/83/1000-0001$03.00/0

model. The idea was enhanced by Swendsen, who obtained very accurate exponents for the static problem through a comparison of normal and renormalized correlation functions, which were calculated from equilibrium configurations generated by Monte Carlo simulations at the critical temperature. The dynamic counterpart to this method was formulated by Tobochnik *et al.*[3] and was used in the analysis of the two,[3,4] and three-dimensional[5] Glauber kinetic Ising model, as well as the Kawasaki kinetic Ising model.[5] This method depends on matching the equilibrium thermodynamic averages obtained from the Monte Carlo configurations and from block spin configurations determined by renormalization; one then searches for times such that the time-dependent averages match. The analysis is complicated and required *good equilibrium* configurations; thus numerous Monte Carlo steps per spin are needed, and only rather small systems like $16 \times 16 \times 16$ in Ref. 5 could be simulated. It is possible that the relatively small lattices considered lead to systematic errors due to boundary and finite size effects. We present below a new dynamical renormalization group which is easier for the computer, more straightforward in the analysis, and allows the simulation of large systems like $128 \times 128 \times 128$ spins; moreover it works also for short times when the system is still relaxing toward equilibrium.

In the next section we describe the method and present the theory. The results for the Glauber and Kawasaki models are presented in Section 3 and these results are compared with those obtained from other methods.

2. METHOD AND THEORY

Consider the system in an initial state at $t = 0$ with all spins parallel: $M(0) = 1$. Through the standard Monte Carlo procedure[6] it is possible to follow the system's relaxation to equilibrium configurations; we choose as the temperature the critical temperature[5] of the model where the correlation length is infinite in an infinite system. The blocking procedure of renormalization group replaces a cell of b^d neighboring spins (in a d-dimensional hypercubic lattice) by one renormalized spin whose sign is, in our case, determined by the majority of original spin orientations in the b^d cell. Let t be the time (in Monte Carlo steps per spin) at which magnetization M of the original system reaches a given value M_1, and let t_b be the time the renormalized system needs to reach the same value M_1 for its renormalized magnetization (which is also unity at the beginning of the simulation). The

[5] The method is dependent on an independent estimation of T_c, e.g., a Monte Carlo analysis or series expansion. An error in T_c will produce systematic errors in z.

dynamic scaling hypothesis asserts that these times are related by

$$t_b = b^z t \tag{1}$$

where $z = \Delta/\nu$ is the dynamical critical exponent we wish to calculate. Alternatively, we can compare the times at which renormalizations of the same original systems reach the same value M_1 of their respective renormalized magnetizations. If these times and length rescaling factors are denoted as t_b and b, or $t_{b'}$ and b', respectively, then

$$t_b/t_{b'} = (b/b')^z \tag{2}$$

The values of z determined in this way should be independent of the choice of the matching magnetization M_1. Consider the simulation of a finite system ($L \times L \times L$) at the critical temperature by Monte Carlo methods, starting with all spins up. The magnetization approaches a metastable finite value of order $L^{-\beta/\nu}$ due to the periodic boundary conditions and the finite size of the system. After a sufficiently long time in this metastable region, the magnetization changes in a relatively short period to zero and then to negative values. From then on it fluctuates in sign. The average time needed for the magnetization to change its sign for the first time is expected at the critical temperature T_c to be proportional to the linear relaxation time, i.e.,

$$\tau_f \propto L^z$$

where τ_f is the flip time, i.e., the time needed for the first reversal of the magnetization after a start from a ground state configuration.

A cell of b^d spins is renormalized to one superspin. This superspin flips its orientation when the magnetization of the cell with b^d spins changes its sign. Thus each superspin flips, on the average, after a time proportional to b^z, if we identify b of the cell with the size L in the argument above and if b is sufficiently large. In this sense one Monte Carlo step for a system of superspins corresponds to about b^z Monte Carlo steps for the original "primary" spins. The normal primary spins in a Monte Carlo simulation need a certain noncritical time in units of one Monte Carlo step per primary spin until one tenth of them are flipped ($M = 0.8$) from the initial "all up" state. This primary flip time does not depend critically on $T - T_c$ or at $T = T_c$ on the system size. The time taken for the primary system to reach a value of the magnetization of 0.8 implies that there should be a delay of a multiplicative factor of b^z time units before the system of superspins reaches the same value of the renormalized magnetization. Thus we have

$$t_b = \text{const} \cdot b^z t \qquad (b \to \infty)$$

Thus a comparison of two different large cells b and b' gives

$$\frac{t_b}{t_{b'}} = \left(\frac{b}{b'}\right)^z$$

the central equation of this method.

This argument can be formulated more quantitatively by defining $P_b(t, T)$ as the probability that an Ising lattice with b^d spins at temperature T in zero magnetic field has a negative magnetization, t Monte Carlo steps per spin after having started with all spins up. (Zero magnetization is counted as negative with probability 1/2 only.) Obviously, $P_b(0, T) = 0$ and $P_b(\infty, T) = 1/2$; for intermediate time s, P_b increases monotonically with t. We are interested here only in the case $T = T_c$. At this critical point, dynamical scaling suggests that $P_b(t, T_c)$ is a scaling function of one variable only:

$$P_b(t, T_c) = f(t/b^z) \qquad (t, b \to \infty)$$

since only one time and one length dominate critical behavior. This assumption should be valid for all probabilities between zero and unity; since probabilities are normalized to unity there is no factor $b^{-\beta/\nu}$ in the above scaling assumption. As long as the system is rather far away from equilibrium the probability P_b is very small or even exactly zero; only for time t where most of the samples lead to an equilibrium magnetization of nearly zero is the probability much larger and close to 1/2.

In our renormalization approach we identify this lattice size b with the cell size b; thus the probability that the majority of spins within a b cell points down equals $f(t/b^z)$. The renormalized magnetization M_b of the system of superspins determined by the majority within each cell is now given by $M_b(t, T_c) = 1 - 2P_b(t, T_c) = 1 - 2f(t/b^z)$ for large b and t. Therefore to every number μ between 0 and 1 belongs one time $t_b(\mu) = \text{const}_\mu \cdot b^z$ such that $M_b[t_b(\mu), T_c] = \mu$. And if we compare two different cell sizes b and b' we have $t_b(\mu)/t_{b'}(\mu) = (b/b')^z$, which is our basic result.

This derivation makes clear that our method does not require to work with equilibrium magnetizations ($\mu = 0$). In principle it works for every positive μ. [The primary spins, however, have to be quite close to equilibrium to give a renormalized magnetization M_b different from unity for large b; in other words, we need $t \to \infty$ if we want to apply the scaling function $f(t/b^z)$ for $b \to \infty$.] On the other hand, P_b must not be defined as the probability to have a magnetization smaller than some positive μ' in our b cell; only $\mu' = 0$ works. If one would take $\mu' = 0.8$, for example, then only 10% of the spins within one cell would have to flip in order to change the cell orientation. This condition is reached after about one Monte Carlo step per spin; thus this time, and the associated probability $P_{b'}$ would not be

critical and would not obey the above scaling relationship. Therefore the usual majority rule ($\mu' = 0$) is required; a smaller number of votes, like 10%, is not sufficient for a change in the orientation.

In summary, our derivation makes clear that we can work with nonequilibrium magnetizations ($\mu > 0$) of our renormalized systems, provided we use the proper majority rule ($\mu' = 0$) within each cell for our renormalization.

3. RESULTS

In Table I we show, for illustration purposes, an example of a 630×630 square Ising lattice, which is renormalized into a 210×210 superlattice of cells; each of these cells contains nine original spins and thus $b = 3$. We replace each 3×3 cell by a single renormalized spin which is taken up as if at least five of the original spins are up; otherwise the superspin is taken as down ("majority rule"). The Monte Carlo simulation is always applied to the original spins, not the renormalized spins, to determine the interaction energies and thermal probabilities. Also, if we take $b = 9$, we determine the sign of the corresponding renormalized spin by the majority of all 81 spins in the 9×9 cell, not by the majority of the nine superspins of the previous 3×3 renormalization. In other words, our majority rule is based on direct, not on representative democracy. In the case of cells with an even number of spins and in which there is no clear

Table I. The Number t and t_b of Monte Carlo Steps per Spin of the Normal and Renormalized System, Shown in the First and Second Column, Which Are Required for the Systems to Reach the Same Value M_1 of the Magnetization Listed in the Third Column[a]

t	t_b	M_1	z
3	27	0.840	2.00
4	38	0.821	2.05
5	47	0.807	2.00
6	64	0.796	2.16
7	74	0.787	2.15
8	85	0.779	2.15
9	92	0.773	2.12

[a] A two-dimensional 3×3 cell is renormalized into one superspin. The dynamic exponent z is calculated as $\log(t_b/t)/\log b$.

majority we assign the renormalized state with probability 1/2, i.e., the state is determined by the "flip of a coin."

The second column in Table I contains the number of Monte Carlo steps per spin required in order that the renormalized system, with $b = 3$, reach the same magnetization as the unrenormalized system at time t. For example, after a time of 27 the 3×3 cells gives us a magnetization of 0.840, which agrees with the magnetization of the unrenormalized system after only three Monte Carlo steps per spin. Therefore, $t_b = 27$, $t = 3$, and thus $z = 2$ since $27 = 3^z \cdot 3$. (For smaller times like $t = 1$ we find that z is small, approximately 1.5, and depends on t. Thus this estimate is unreliable.) Our two-dimensional data are based on 100 Monte Carlo steps per spin in a 630×630 lattice, using the standard algorithm.[6] In Table II we show the z obtained for various rescaling factors b and b', and averaged over suitable values for the matching magnetization M_1. (Also we averaged over 32 different simulations.) The mean value of the z exponents in Table II is 2.12, with a statistical error of 0.06.

Larger systems were simulated over longer times for three dimensions. Figure 1 shows our original and renormalized magnetizations, with $b = 1$, 2, 4, 8, 16, and 32, calculated from a 128×128 simple cubic lattice. We made six simulations up to 100 Monte Carlo steps per spin, two up to 300, and, in addition, we have completed four runs up to $t = 1000$ for a $128 \times 128 \times$

Table II. Exponent Estimates for the Two-Dimensional z[a]

b	b'	z
1	3	2.09
1	4	2.05
1	5	2.05
2	3	2.60
2	4	2.36
3	4	2.00
3	6	2.04
4	5	2.10
4	8	2.03
5	6	1.95
6	7	2.06

[a] Cells of size $b \times b$ and of size $b' \times b'$ are renormalized into one superspin each, and compared with each other. The exponent z is calculated as $\log(t_b/t_{b'})/\log(b/b')$.

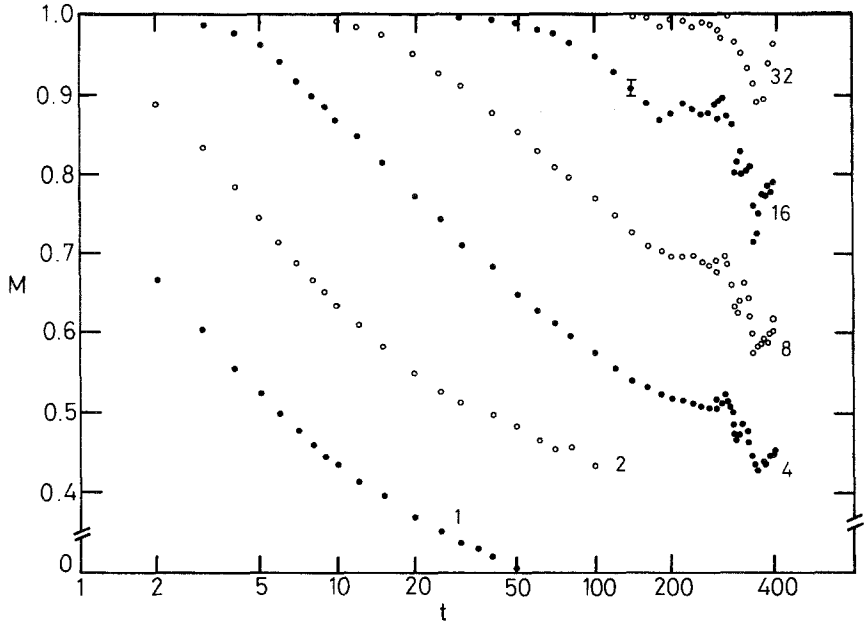

Fig. 1. Variation of the original magnetization and of the renormalized magnetizations with time, i.e., with the number of Monte Carlo steps per spin in the original system. Because of our logarithmic time scale, the similarity assumption on which our approach is based means that these curves can be made to coincide by shifts to the right or left. The numbers on the data sets give b, the length rescaling factor.

128 lattice. The results for times up to 500 confirm the values reported here. However, for t above 500 the magnetization decayed only very weakly with time; finite-size effects become more pronounced and thus the data are unreliable. Larger lattices seem necessary to get more reliable information for t of the order of 1000. One such Monte Carlo step per spin took 10.8 sec on our IBM 370/168 including the renormalization analysis.[6] Only 11% of the computer time and less than 2% of the memory were used for the renormalization part; the rest was spent with producing the configurations by multispin coding.[7] (The results for $b = 2$ were obtained by 20 runs on a $64 \times 64 \times 64$ lattice up to 100 Monte Carlo steps per spin.) Except for times larger than 100, the Monte Carlo error is of the order of the symbol size in our figure.

Our renormalization method requires that the curves for different b in Fig. 1 can be made to coincide by a rescaling of the time, i.e., by a simple

[6] Calculations for larger lattices on a CDC Cyber 205 vector computer are planned by C. Kalle, Ref. 7.

Table III. Exponent Estimates for the Three-Dimensional z

b'	b: 1	2	4	8	16
2	2.07				
4	2.20	2.36			
8	2.16	2.12	2.20		
16	2.17	2.11	2.04	2.20	
32	2.01	1.99	2.00	2.06	2.14

[a] Cells of size b^3 and of size b'^3 are renormalized into one superspin each, and compared with each other. The exponent z is calculated as $\log(t_b/t_{b'})/\log(b/b')$.

shift to the right or left in our logarithmic plot. For longer times, the data for $b = 1$ cannot be made to match those for larger b; similarly but weaker, the same difficulty occurs with $b = 2$. But for $b = 4$ and larger cells, the different curves can be made to coincide approximately by such a time rescaling, as the reader may check by superimposing two copies of this figure. Thus, our real space renormalization is not exact for small cells, which is hardly surprising,[8] but works better for larger cells. And only for long times can we see the deviations for small cells.

Table III gives the resulting estimates for the three-dimensional z, with each single value having an error of the order 0.1. There seems to be a systematic trend toward smaller z if we compare two cells with drastically different b and b'. But renormalization is expected to work best for a constant ratio b/b' of order unity. Thus this systematic trend with varying b/b' should not lead us to extrapolate z to values lower than those in the table. At fixed b/b', our Table III gives no indication of a systematic trend with increasing b (in principle we are interested in the $b \to \infty$ limit only). This answers one of the crucial questions left open by earlier real space renormalizations for much smaller systems; cell size effects in this type of renormalization seem to be quite small once b is at least 4.

The average over all 15 estimates in Table III is $z = 2.12$; it does not change if we omit the four values involving $b = 1$; and it shifts only to $z = 2.11$ if we also omit the three values with $b = 2$. The statistical error is about 0.03 in all three cases. Therefore, if we can trust our conclusion that no systematic trends with increasing b at constant b/b' shift the asymptotic exponent away from our estimates, then

$$z = 2.11 \pm 0.03$$

seems a realistic estimate for three dimensions.

We also made an analysis involving short times up to 100 Monte Carlo steps per spin, with a program similar to our two-dimensional analysis, for

$60 \times 60 \times 60$ lattices. The average of six different z estimates, involving pairs $(b, b') = (1,3)$; $(1,4)$; $(1,5)$; $(2,4)$; $(3,6)$; and $(4,8)$, was found to be 2.07 ± 0.03, giving more credence to the consistency of our method and indicating that good accuracy can be obtained already with systems of moderate size and shorter observation time.

We now describe the application of this method to the two-dimensional Kawaski Ising model[10,11] in which the order parameter, the magnetization, but not the energy, is conserved. In the usual Kawasaki model, relaxation is achieved by interchanging a random spin with one of its (randomly selected) nearest neighbors of opposite spin orientation, thus ensuring the conservation of the magnetization. The approach of this system to equilibrium at the critical temperature, T_c, is much slower than that of the Glauber model, in which neither the energy nor the order parameter is conserved. A consequence of this is that previous analyses of the Kawaski dynamical model by MCRG[5] have been restricted to very small system with the danger of unavoidable large finite size effects. The model, however, may be brought to equilibrium more rapidly by the inclusion of further neighbors in the exchange process. We refer to this system as the generalized Kawasaki model. We expect from general considerations that the dynamic critical properties of this system should be in the same universality class as the Kawasaki model and indeed, this has been confirmed by our results. The initial system comprised a random arrangement of spins in which the net magnetization was zero. In Table IV we show our results for a system of 300×300 spins both for the usual and the extended Kawasaki models. In each case the results can be determined

Table IV. Exponent Estimates for the Two-Dimensional z

b'	$b \rightarrow$	3	4
2		3.42	3.90
		3.71	4.32
3			4.25
			3.82

[a] Cells of size $b \times b$ and of size $b' \times b'$ are renormalized into one superspin each, and compared with each other. The exponent z is calculated as $\log (t_b/t_{b'})/\log(b/b')$. The upper values are calculated for the usual Kawasaki model, and the lower for the generalized model involving exchange between fifth nearest neighbors.

from only 1000 Monte Carlo steps per spin. The complete run took 70 min on an IBM 370/168 computer.

4. CONCLUSION

Our two-dimensional $z = 2.12 \pm 0.06$ (probable error not maximum error!) agrees reasonably with earlier estimates of 2.17 in Ref. 3 and 2.22 in Ref. 4 and is consistent with less accurate estimates from Monte Carlo simulations above[6,11] and at T_c. Our three-dimensional $z = 2.11 \pm 0.03$ agrees well with the Monte Carlo renormalization result $z = 2.08$ of Ref. 5 though our estimate seems to be more accurate. It is also consistent with $z = 2.17 \pm 0.06$ obtained from Monte Carlo simulation above T_c using much more computer time[13]; but it seems to be slightly higher and outside the range of $z = 2.02$ as found[14] by interpolation between two epsilon expansions. For the Kawasaki model we obtain a value of 3.9 ± 0.1 which is somewhat higher than the expected result of 3.75, derived from the relation

$$Z = 4 - \eta$$

as obtained by Halperin, Hohenberg and Ma.[15] We speculate that this may be due to the effects of finite system size which would tend to place the value of η between the mean field result of 0 and exact result of 0.25. It would be interesting to test this conjecture by examining larger systems with this method.

In summary, our method requires a much simpler analysis than previous methods and thus allowed for the use of larger systems and a search for finite-size effects. The method is simple enough to consider the application to the evaluation of z for other systems.

ACKNOWLEDGMENTS

The Center for Polymer Studies is supported in part by grants from ARO, NSF, and ONR. We thank H. J. Herrmann for critical discussions and A. Aharony, R. Folk, W. Klein and A. Zippelius for helpful suggestions.

REFERENCES

1. S. K. Ma, *Phys. Rev. Lett.* **37**:461 (1976).
2. R. H. Swendsen, *Phys. Rev. Lett.* **42**:859 (1979); R. H. Swendsen, in *Real Space Renormalization*, T. W. Burkhardt and J. M. J. Van Leeuwen, eds. (Topics in Current Physics, Vol. 30, Springer, Heidelberg, 1982), p. 57; G. F. Mazenko and O. T. Valls, ibid., page 87.

3. J. Tobochnik, S. Sarker, and R. Cordery, *Phys. Rev. Lett.* **46**:1417, (1981).
4. S. L. Katz, J. D. Gunton, and C. P. Liu, *Phys. Rev. B* **25**:6008 (1982).
5. M. C. Yalabik and J. D. Gunton, *Phys. Rev. B* **25**:534 (1982).
6. K. Binder, ed., *Monte Carlo Methods in Statistical Physics* (Topics in Current Physics, Vol. 7, Springer, Heidelberg, 1979).
7. R. Zorn, H. J. Herrmann, and C. Rebbi, *Comp. Phys. Comm.* **23**:337 (1981); C. Kalle and V. Winkelmann, *J. Stat. Phys.* **28**:639 (1982).
8. P. J. Reynolds, H. E. Stanley, and W. Klein, *Phys. Rev. B* **21**:1223 (1980).
9. K. Kawasaki, *Phys. Rev.* **145**:223 (1965).
10. K. Kawasaki, in *Phase Transitions and Critical Phenomena*, Vol. 2, C. Domb and M. S. Green, eds. (Academic, New York, 1972).
11. N. Jan and D. Stauffer, *Phys. Lett.* **93A**:39 (1982).
12. J. C. Angles d'Auriac, R. Maynard, and R. Rammal, *J. Stat. Phys.* **28**, 307 (1982).
13. C. K. Chakrabarti, H. G. Baumgärtel, and D. Stauffer, *Z. Phys. B* (*Cond. Matter*) **44**:333 (1981).
14. R. Bausch, V. Dohm, H. K. Janssen, and R. K. P. Zia, *Phys. Rev. Lett.* **47**:1837 (1981).
15. B. I. Halperin, P. C. Hohenberg, and S. K. Ma, *Phys. Rev. B* **10**:139 (1974).