Monte Carlo renormalization-group study of the impure Baxter-Wu model

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We have used a Monte Carlo renormalization-group method to study the Baxter-Wu model with random, quenched, nonmagnetic site impurities. The results clearly show that the impurities change the critical exponents from the zero-impurity exact value of $\nu=\frac{2}{3}$ to $\nu=0.97\pm0.04$. The magnetic and crossover exponents do not change measurably with the addition of the impurities. We also find that the fixed point for the model with quenched impurities is further from the starting Hamiltonian than it was for the pure model.

I. INTRODUCTION

The effects quenched impurities have on the critical behavior of $d=2$ magnetic systems have been the subject of several studies in recent years.[1-8] One motivation for these studies is that in experiments some measure of fixed impurities is always present. Hence the theoretical study of quenched (fixed) impurities is of importance to the understanding of physical experiments.[2] Using general arguments Harris[1] suggested that the effects of quenched impurities were determined by the value of the specific-heat exponent α of the pure system. If $\alpha<0$ then the quenched impurities should change the critical temperature T_c but should not change the critical exponents. If $\alpha>0$ then the addition of random quenched impurities should change the critical exponents as well as T_c. Studies of an m-component continuous spin model using renormalization-group (RG) methods[3] showed that if $\alpha>0$ (and not if $\alpha<0$) the addition of random quenched impurities make a new "random" fixed point stable. Exact work using transfer matrices on the rectangular Ising model[4] ($\alpha=0$) showed that quenched, periodic point defects changed T_c but not the critical exponents. Monte Carlo (MC) simulations for $d=2$ Ising models with quenched random site impurities found no change in the critical exponents.[5] A study of the Baxter-Wu model ($\alpha=\frac{2}{3}$) used finite-size scaling to analyze MC data and demonstrated that the static critical exponents did change with the addition of random quenched site impurities.[6] A recent MC study of the dynamics of the Baxter-Wu model provided evidence that the dynamic exponents also change when random quenched site impurities are present.[7] In this paper we report on a Monte Carlo renormalization-group (MCRG) study of the Baxter-Wu model with quenched random nonmagnetic site impurities, and obtain the associated critical exponents.

The rest of the paper is organized as follows. Section II contains background information with a brief introduction to the Baxter-Wu model in Sec. II A and a description of the MCRG method in Sec. II B. Section III contains our results. Discussions and conclusions are presented in Sec. IV.

II. BACKGROUND

A. The Baxter-Wu model

The Baxter-Wu model is a simple model consisting of Ising spins with three-body interactions on a triangular lattice. The Hamiltonian is given by

$$\mathscr{H}=-J\sum_{i,j,k}{}'\sigma_i\sigma_j\sigma_k\ , \tag{1}$$

where $\sigma_i=\pm1$ and the prime on the summation indicates that the sum is over all triangles made from nearest-neighbor spins on the lattice. In the locations of a random quenched (fixed) nonmagnetic site impurity, $\sigma=0$. In the absence of any applied field, the ground state is fourfold degenerate. A triangular lattice is composed of three triangular sublattices, and in the ground state all spins on a sublattice are either up or down. One ground state is ferromagnetic with all spins up, and the other three are ferrimagnetic which have spins on one sublattice up and spins on the other two sublattices down (see Fig. 1). An exact solution by Baxter and Wu for the pure model (where the fraction of random quenched site impurities $x=0$) gave the critical temperature $kT_c(0)/J=2/\ln(\sqrt{2}+1)\approx2.2692$ and the critical exponents $\nu=\nu'=\alpha=\alpha'=\frac{2}{3}$. Hence the exact value of the thermal exponent for the pure model is $y_T=1/\nu=\frac{3}{2}$. Series expansions gave the magnetic susceptibility $\gamma_M=1.17$ (Refs. 10 and 11) and a conjecture for the spontaneous magnetization M with exponent $\beta_M=\frac{1}{12}$.[11] Hence series analysis and scaling yield a magnetic exponent for the pure lattice of $y_H=1.875$. For the pure system, Barber[12] has shown that corrections to the asymptotic power-law behavior require a third relevant exponent $y_3=\frac{7}{8}$ (Barber assumed $y_H=\frac{15}{8}$ as in the $d=2$ Ising model and used the exact value $y_T=\frac{3}{2}$). Real-space RG

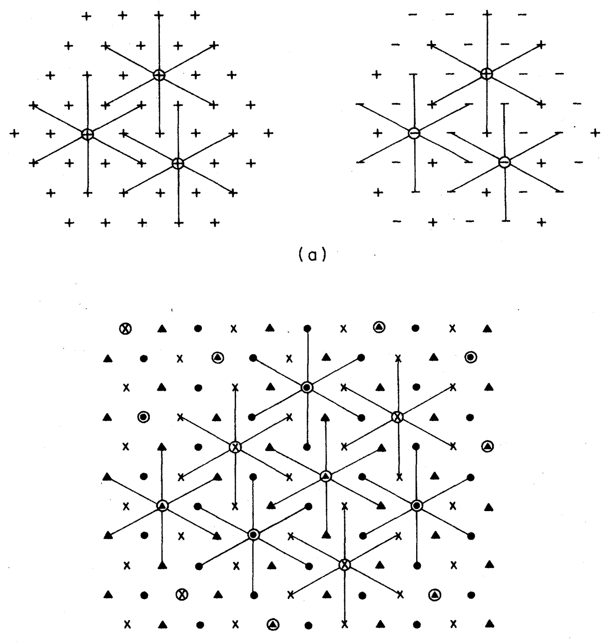

FIG. 1. (a) Ferromagnetic and one of the ferrimagnetic ground states are shown, together with the seven spins that are used to obtain a block spin for the $b=\sqrt{7}$ transformation. (b) The three triangular sublattices are indicated by $\times$, ▲, and ●. The block spins that make up the renormalized lattice are indicated by the circled symbols.

methods have also been used to study the pure Baxter-Wu model and have found three exponents,[13] but the values obtained for the exponents are not in good agreement with the exact solutions and series estimates. A MCRG study of the pure Baxter-Wu model[14] obtained three relevant eigenvalues which were in good agreement with the exact and conjectured values.

A MC study of the Baxter-Wu model for the pure case ($x=0$) and for different fractions x of nonmagnetic random site impurities has been reported previously.[6] This study used finite-size scaling to analyze the data, and showed a dramatic change in the critical exponents to $\nu=1.00\pm0.07$ and $\gamma_M=1.95\pm0.08$ for all nonzero impurity concentrations studied (values of x between 0.028 and 0.222 were included). In Sec. III we will present our MCRG study of the Baxter-Wu model with $x=0.111$ which will confirm the exponent values obtained from finite-size scaling. First we briefly describe the MCRG method.

B. The MCRG method

We use the MCRG method[15,16] which was successful in reproducing the critical exponents in the pure Baxter-Wu model.[14] We perform MC simulations on $L\times L$ triangular lattices with periodic boundary conditions using the method outlined elsewhere.[6] On the $L\times L$ spin configurations generated using the MC, a real-space RG with a scale factor b is performed to obtain a block spin from each distinct set of b^2 spins. This gives block spin configurations on $L/b\times L/b$ lattices which are governed by the exact renormalized Hamiltonian. Further RG transformations reduce the lattice size by additional factors of b and yield block spin configurations on these lattices. The critical exponents are obtained from the linearized transformation matrix

$$T_{\alpha\beta}=\frac{\partial K_\alpha^{(n)}}{\partial K_\beta^{(n-1)}}\,, \tag{2}$$

where $K_\alpha^{(n)}$ is the coupling constant corresponding to the spin operator S_α following the nth RG transformation. (The K_α include factors of $1/kT$.) From the chain rule

$$\frac{\partial[\langle S_\gamma^{(n)}\rangle]}{\partial K_\beta^{(n-1)}}=\sum_\alpha T_{\alpha\beta}\frac{\partial[\langle S_\gamma^{(n)}\rangle]}{\partial K_\alpha^{(n)}}\,, \tag{3}$$

where the angular brackets indicate a thermal average for a particular distribution of quenched impurities and the square brackets indicate the average over all different impurity distributions. The partial derivatives can be calculated from the canonical ensemble for a system with quenched variables:[17]

$$\frac{\partial[\langle S_\gamma^{(n)}\rangle]}{\partial K_\alpha^{(m)}}=[\langle S_\gamma^{(n)}S_\alpha^{(m)}\rangle-\langle S_\gamma^{(n)}\rangle\langle S_\alpha^{(m)}\rangle]\,. \tag{4}$$

The quantities on the right-hand side of Eq. (4) are calculated from the spin and block spin configurations in the normal MC fashion.[18] In particular, the thermal averages $\langle\ \rangle$ are first calculated by averaging over all spin sites and all MC spin configurations, and then the quenched averages [ ] are calculated by averaging the thermal averages over a number of different distributions of the quenched variables.

To yield accurate critical exponents the RG transformation should preserve the symmetry of the Hamiltonian.[9] For this reason, we have used a transformation with a scale factor of $b=\sqrt{7}$. This transformation uses a majority rule to form a block spin from a center spin and its six nearest-neighbor spins on the same triangular sublattice. If the sum $\mathscr{S}$ is zero, an impurity ($\sigma=0$) was placed on that lattice site. Note that the first transformation yields a rotated lattice with skew boundary conditions, and the next transformation gives an unrotated lattice with normal periodic boundary conditions. This real-space RG transformation is illustrated in Fig. 1. (Other transformations placing an impurity on the renormalized lattice if the sum with $|\mathscr{S}|\le1$ and $|\mathscr{S}|\le2$ gave results comparable to those presented below.)

III. RESULTS

This MCRG study was performed at three temperatures on a 147×147 triangular lattice with periodic boundary conditions. The simulations were performed only with a fraction $x=0.111$ of random, quenched, nonmagnetic site impurities. The thermalization for each temperature and impurity configuration was accomplished by initially throwing away 15 000 Monte Carlo steps per spin (MCS) from a starting configuration of random spins. The MCRG analysis then used 10^5 MCS, with the RG transformation performed on spin configurations separat-

TABLE I. The thermal, magnetic, and crossover exponents obtained from the MCRG are shown. The simulation was performed at $kT/J=1.62$ for two different distributions of quenched impurities on a 147×147 lattice.

Iteration	Coupling constants	y_T	y_H	y_3
1	1		1.746	
	2	0.400	1.763	
	3	0.670	1.763	
	4	0.671	1.765	
	5	0.705	1.764	
	6	0.720	1.764	
	7	0.682	1.762	
	8	0.677	1.762	
	9	0.676	1.762	
	10		1.760	
2	1	0.051	1.774	
	2	0.982	1.848	0.271
	3	1.091	1.843	0.550
	4	1.106	1.838	0.633
	5	1.081	1.839	0.662
	6	1.071	1.840	0.671
	7	1.034	1.826	0.749
	8	1.029	1.825	0.754
	9	1.025	1.827	0.751
	10		1.828	0.714
3	1		1.627	
	2	0.772	1.841	0.288
	3	0.965	1.853	0.458
	4	1.051	1.843	0.585
	5	0.989	1.851	0.655
	6	0.945	1.847	0.657
	7	1.053	1.816	0.678
	8	1.057	1.814	0.747
	9	1.047	1.808	0.740
	10		1.813	0.680

TABLE II. The thermal, magnetic, and crossover exponents obtained from the MCRG are shown. The simulation was performed at $kT/J=1.60$ for one distribution of quenched impurities on a 147×147 lattice. The RG flows show that this temperature is below T_c.

Iteration	Coupling constants	y_T	y_H	y_3
1	1		1.762	
	2	0.337	1.771	
	3	0.646	1.771	0.125
	4	0.652	1.771	0.123
	5	0.696	1.770	0.132
	6	0.718	1.771	0.110
	7	0.648	1.769	0.153
	8	0.622	1.769	0.161
	9	0.622	1.768	0.124
	10		1.763	0.173
2	1		1.820	
	2	0.759	1.883	0.172
	3	0.958	1.891	0.547
	4	0.989	1.888	0.647
	5	0.964	1.894	0.678
	6	0.951	1.892	0.644
	7	0.887	1.885	0.751
	8	0.884	1.885	0.753
	9	0.884	1.886	0.724
	10		1.887	0.708
3	1		1.756	
	2	0.001	1.999	
	3	0.522	2.027	0.176
	4	0.575	1.977	0.354
	5	0.510	1.991	0.400
	6	0.510	1.990	0.443
	7	0.512	1.966	0.579
	8	0.469	1.964	0.620
	9	0.461	1.929	0.500
	10		1.915	0.490

ed by 20 MCS. Tables I—III show 3 RG transformations between lattices with linear dimensions: $147\rightarrow21\sqrt{7}$, $21\sqrt{7}\rightarrow21$, and $21\rightarrow3\sqrt{7}$. Another RG transformation to a 3×3 lattice was also performed, but on this small lattice finite-size effects were very apparent. Hence this last RG iteration is not shown in the tables. The nine even operators (which have $[\langle S_\alpha\rangle]\neq0$) and the ten odd operators (which have $[\langle S_\alpha\rangle]=0$) used in the RG analysis are shown in Fig. 2. The first even operator is a "fugacity" for the quenched impurities, while all other operators include the signs of the spins. Only one distribution of the site impurities was used for $kT/J=1.60$ and 1.65, while two different random distributions of the site impurities were used at $kT/J=1.62$. Both impurity distributions for $kT/J=1.62$ were also analyzed separately, and gave results comparable to those obtained using two distributions. Thus for this lattice size, it is more important to have adequate thermal averages than to average over a number of different distributions of the impurities. (However when this MCRG was performed on 42×42 lattices it was found that averaging over at least 20 different distributions of the site impurities was necessary. This should be expected since for larger lattice sizes a larger number of local impurity distributions are sampled than for a smaller size lattice.)

The convergence of the eigenvalues obtained from the MCRG for our best estimate of $kT_c/J=1.62$ are shown in Table I. For the first RG iteration all three exponents have significantly different values than they do for the last two iterations. In fact y_3 is absent entirely in the first iteration. This shows that the RG is not yet within the linear region about the fixed point after the first iteration. Consequently the first iteration should not be used to obtain eigenvalue estimates. This contrasts with the MCRG study of the pure Baxter-Wu model[14] where the exponents after the first iteration had already converged. Consequently the "impure" fixed point is further from the starting Hamiltonian than is the pure fixed point. For the thermal exponent y_T the eigenvectors of $T_{\alpha\beta}$ showed that the "impurity fugacity" did not have an important contribution to the RG flows. We also found that operators 2,

TABLE III. The thermal, magnetic, and crossover exponents obtained from the MCRG are shown. The simulation was performed at $kT/J=1.65$ for one distribution of quenched impurities on a 147×147 lattice. The RG flows show that this temperature is above T_c.

Iteration	Coupling constants	y_T	y_H	y_3
1	1		1.744	
	2	0.394	1.756	
	3	0.696	1.756	
	4	0.697	1.755	
	5	0.715	1.754	
	6	0.725	1.754	
	7	0.650	1.752	
	8	0.649	1.750	
	9	0.651	1.751	
	10		1.748	
2	1		1.755	
	2	0.715	1.804	0.328
	3	0.937	1.803	0.489
	4	0.961	1.804	0.528
	5	0.933	1.804	0.539
	6	0.912	1.806	0.535
	7	0.881	1.802	0.541
	8	0.890	1.806	0.546
	9	0.892	1.812	0.516
	10		1.817	0.486
3	1		1.586	
	2	0.103	1.720	0.322
	3	0.331	1.738	0.391
	4	0.391	1.734	0.391
	5	0.267	1.744	0.390
	6	0.271	1.744	0.402
	7		1.717	0.291
	8		1.719	0.264
	9		1.714	0.218
	10		1.711	0.211

3, and 4 all had significant (greater than 10%) contributions to the eigenvector associated with y_T. Thus the values for y_T should only be considered when at least four even operators are included. We thus obtain a value of $y_T=1.03\pm0.04$ from the MCRG results. This result is in agreement with finite-size scaling analysis of MC data[6] which found $y_T=1/\nu=1.00\pm0.07$. Finite-size scaling analysis of MC data[6] and a MCRG study[14] of the pure model both found thermal exponents consistent with the exact pure lattice value of $y_T=\frac{3}{2}$.[9] Hence the dramatic change in the thermal exponents when quenched impurities are present is seen in both studies. Thus the transition remains second order, but the presence of the quenched impurities changes the thermal exponent. The eigenvectors of $T_{\alpha\beta}$ associated with the magnetic exponent y_H showed significant contributions only from the first two odd operators, which are associated with the two order parameters of the model.[11] Table I gives a value for y_H which is smaller than the pure model of 1.875. However, the value of y_H is extremely sensitive to the simulation

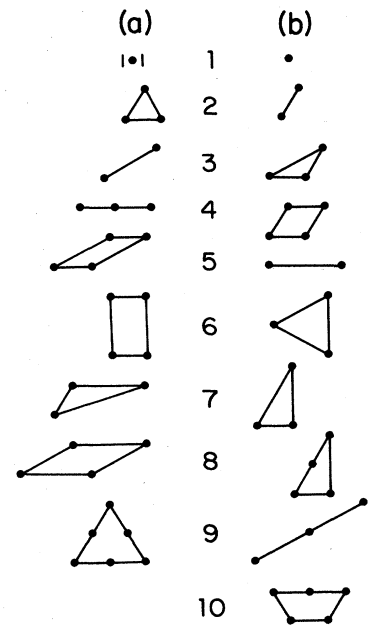

FIG. 2. (a) The 9 even and (b) the 10 odd spin operators used in the study are shown.

temperature, as we will demonstrate below. Consequently the impure value for y_H may be unchanged from the pure lattice value. A third relevant operator y_3 associated with the odd operators is clearly evident in the last two iterations in Table I. y_3 is significantly below the pure model value of 0.875 found from corrections to scaling,[13] a value also consistent with the MCRG study of the pure lattice.[14]

Table II shows the eigenvalues at a temperature of $kT/J=1.60$ and Table III shows the eigenvalues at $kT/J=1.65$. These tables are used to support the temperature $kT/J=1.62$ as being near T_c, and to provide estimates of the errors for the exponents. The first iteration in both Tables II and III is not within the linear regime of the "impure" fixed point and should be ignored. Table II shows that $T=1.60$ is below T_c. The second iteration has come close to the linear region of the "impure" fixed point, but the next iteration flows toward the trivial $T=0$ discontinuity fixed point ($y_H=d=2$). Table III shows that $T=1.65$ is above T_c. The flows are first attracted toward the impure fixed point, but then flow toward the trivial $T=\infty$ fixed point. In fact, y_T ceases to become relevant in the last iteration once more than six operators are present. The flows for these three temperatures are shown schematically in Fig. 3. Note that y_H increases as T decreases, while y_T and y_3 both go through a maximum at T_c. This shows that if T_c were slightly below $T=1.62$ the value of y_H found might correspond to the infinite lattice value of 1.875. Thus we find $y_H=1.85\pm0.04$, which includes the pure lattice value. The systematic error due to the uncertainty in T_c is not as large for y_T or y_3. Hence the errors in the value of y_T obtained at $T=1.62$ do not have to be increased due to the error in T_c. For y_3 the largest error is from biased estimation due to the nature of the functions which must be

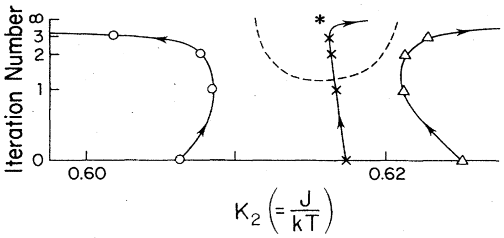

FIG. 3. RG flows for each of the three temperatures simulated are shown schematically. The horizontal axis represents the J/kT axis (the spin operator in the simulated Hamiltonian), and the vertical axis is the RG iteration number. The region inside the dashed curve is the linear regime about the fixed point (*). $\triangle$, $\times$, and $\circ$ indicate schematically the position on the flow lines after each application of the RG transformation for temperatures of 1.60, 1.62, and 1.65, respectively.

calculated from the MC data. This source of error in y_3 was evident when we analyzed only a portion of the MC data, and when we performed a b^2 transformation. These warning signs make it impossible at present to give a value for y_3.

The RG flows discussed above give a value of $1.60 < kT_c/J < 1.65$, which is consistent with the value from finite-size scaling of MC data ($kT_c/J = 1.60 \pm 0.05$).[6] We tried to obtain T_c from the extended MCRG method.[19] This method compares spin operators on same size lattices which have undergone a different number of RG transformations. We used this method on lattices with initial linear dimensions of 42 and $6\sqrt{7}$. Since after the first iteration the RG flows are still not within the linear regime of the impure fixed point, we were only able to obtain accurate estimates for T_c on the 6×6 lattices. This gave estimates of T_c consistent with $T_c = 1.62$, but which had error estimates larger than those we could determine using the RG flows. Use of larger lattices within the extended MCRG method could not obtain thermal averages accurate enough to obtain better estimates for T_c with reasonable amounts of computer time. Consequently, we have obtained T_c from the RG flows indicated in the three tables.

IV. DISCUSSION AND CONCLUSIONS

This MCRG study illustrates that the presence of random, quenched, nonmagnetic site impurities in the Baxter-Wu model dramatically changes the thermal exponent. The pure Baxter-Wu model has $\nu = \frac{2}{3}$, and we find the impure model to have $\nu = 0.97 \pm 0.04$. This MCRG study was performed only at a fraction $x = 0.111$ of impurities. However, the concentration of quenched impurities have been found to not change the critical exponents,[3,6] but only to change the width of the crossover region.[1,6] A parallel MCRG study of the $d = 2$ Baxter model has found that the critical exponents for the pure model with positive values of α in the presence of quenched impurities are pure $d = 2$ Ising exponents within the errors.[8] (The Baxter model was studied at pure model values of $\alpha = 0.372$ and 0.491.[8]) There exists an exact mapping between the Baxter-Wu model and the Baxter model.[20] (The mapping is exact except for boundary conditions and the site impurities.) Hence the present study can be interpreted as an additional data point for the Baxter model which has the particular coupling which has a pure model value of $\alpha = \frac{2}{3}$. In conclusion, we have presented additional evidence that for all $d = 2$ pure models that have $\alpha > 0$ the addition of quenched random impurities changes the magnetic and thermal exponents to close to, if not equal to, those of the pure $d = 2$ Ising model.

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[1]A. B. Harris, J. Phys. C **7**, 1671 (1974).

[2]L. D. Roelofs, A. R. Kortan, T. L. Einstein, and R. L. Park, Phys. Rev. Lett. **46**, 1465 (1981); **47**, 1348 (1981).

[3]A. B. Harris and T. C. Lubensky, Phys. Rev. Lett. **33**, 1540 (1974); T. C. Lubensky, Phys. Rev. B **11**, 3573 (1975); D. H. Khmelnitskii, Zh. Eksp. Teor. Phys. **68**, 1960 (1975) [Sov. Phys.—JETP **41**, 981 (1976)]; G. Grinstein and A. Luther, Phys. Rev. B **13**, 466 (1976); A. Aharony, Y. Imry, and S.-K. Ma, *ibid.* **13**, 466 (1976); C. Jayaprakash and H. J. Katz, *ibid.* **16**, 3987 (1977).

[4]M. E. Fisher and H. Au Yang, J. Phys. C **8**, L418 (1975); Phys. Rev. B **13**, 1238 (1976); **13**, 1266 (1976).

[5]W. Y. Ching and D. L. Huber, Phys. Rev. B **13**, 2962 (1976); E. Stoll and T. Schneider, in *Magnetism and Magnetic Materials—1975, Philadelphia,* proceedings of the 21st Annual Conference on Magnetism and Magnetic Materials, edited by J. J. Becker, G. H. Lander, and J. J. Rhyne (AIP, New York, 1976), Vol. 29, p. 490; R. Fisch and A. B. Harris, *ibid.*, Vol. 29, p. 488.

[6]M. A. Novotny and D. P. Landau, Phys. Rev. B **24**, 1468 (1981); J. Magn. Magn. Mater. **15-18**, 247 (1980).

[7]M. A. Novotny and D. P. Landau (unpublished).

[8]D. Matthews-Morgan, D. P. Landau, and R. H. Swendsen, Phys. Rev. Lett. **53**, 679 (1984).

[9]R. J. Baxter and F. Y. Wu, Phys. Rev. Lett. **31**, 1294 (1973); Aust. J. Phys. **27**, 357 (1974); R. J. Baxter, *ibid.* **27**, 368 (1974).

[10]H. P. Griffiths and D. W. Wood, J. Phys. C **6**, 2533 (1973); D. W. Wood and H. P. Griffiths, *ibid.* **7**, 1417 (1974).

[11]M. G. Watts, J. Phys. A **7**, L85 (1974); M. F. Sykes and M. G. Watts, *ibid.* **8**, 1469 (1975); R. J. Baxter, M. F. Sykes, and M. G. Watts, *ibid.* **8**, 245 (1975).

[12]M. N. Barber, J. Phys. A **9**, L171 (1976).

[13]H. J. Braathen and P. C. Hemmer, Phys. Norv. **8**, 69 (1975);

D. Imbro and P. C. Hemmer, Phys. Lett. **57A**, 297 (1976); M. P. M. den Nijs, A. M. M. Pruisken, and J. M. J. van Leeuwen, Physica (Utrecht) **84A**, 539 (1976); N. Jan, Can. J. Phys. **59**, 708 (1981).

[14]M. A. Novotny, D. P. Landau, and R. H. Swendsen, Phys. Rev. B **26**, 330 (1982).

[15]R. H. Swendsen, Phys. Rev. Lett. **42**, 859 (1979).

[16]R. H. Swendsen, *Real Space Renormalization,* Vol. 30 of *Topics in Current Physics,* edited by T. W. Burkhardt and J. M. J. van Leeuwen (Springer, Berlin, 1982).

[17]S.-K. Ma, *Modern Theory of Critical Phenomena* (Benjamin, Reading, Mass., 1976).

[18]K. Binder, *Monte Carlo Methods in Statistical Physics* (Springer, Berlin, 1979).

[19]D. P. Landau and R. H. Swendsen, Phys. Rev. Lett. **46**, 1437 (1981). Both this extended MCRG method as well as another, less powerful method [S. H. Shenker and J. Tobochnik, Phys. Rev. B **22**, 4462 (1980)] have been attributed to unpublished works of K. Wilson.

[20]R. J. Baxter and I. G. Enting, J. Phys. A **9**, L149 (1976).