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Monte Carlo Renormalization Group and Ising Models with $n \geqslant 2$

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We suggest that the Monte Carlo renormalization group, when combined with the type of cell-spin transformation introduced by van Leeuwen, should be a powerful tool in the study of Ising models with $n \geqslant 2$. Numerical results are presented for the Baxter model and the Ising model with nearest– and next-nearest–neighbor interactions on a square lattice.

The suggestion of Ma[1] to combine the ideas of the renormalization group[2] with Monte Carlo simulations has recently been carried forward by the development of a new calculational approach.[3,4] Results obtained encourage the belief that the Monte Carlo renormalization group (MCRG) has wide applicability in the study of phase transitions. The method has yielded reliable approximations to transition temperatures and critical indices, and has been able to distinguish first-order from continuous transitions. In particular, the critical exponents of the nearest-neighbor Ising model in two[3,4] and three[5] dimensions have been calculated in good agreement with known results. Moreover, the three-component Potts model has been studied in two,[3] three,[6] and four[6] dimensions. In two dimensions a continuous transition was found as expected,[7] while in three and four dimensions the transition was determined to be first order.

In this note we emphasize that the MCRG, when combined with the type of cell-spin transformation introduced by van Leeuwen,[8] should be a powerful tool in the study of Ising antiferromagnets whose phase transitions are described by order parameters having $n \geqslant 2$ components.[9] The specific calculations reported here are for the Baxter model,[10] and for the Ising model with nearest-neighbor (nn) and next-nearest–neighbor (nnn) interactions on a square lattice. The Hamiltonian for the Baxter model is[11] ($K_2 > 0$)

$$H_{\mathrm{B}} = -K_2 \sum_{\mathrm{nnn}} S_i S_j - K_4 \sum_{\langle ijkl \rangle} S_i S_j S_k S_l, \tag{1}$$

where a factor of $1/kT$ has been absorbed in the K_i; $S_i = \pm 1$; the first summation is over nnn pairs and the second is over spins lying at the four vertices of a square. The Ising Hamiltonian is

$$H_{\mathrm{I}} = -K_1 \sum_{\mathrm{nn}} S_i S_j - K_2 \sum_{\mathrm{nnn}} S_i S_j. \tag{2}$$

It is convenient to divide the lattice into two sublattices A and B such that nearest neighbors of spins in A are in B, and vice versa. The two components of the Baxter model's order parameter are the A- and B-sublattice magnetizations. When

$$-2K_2 > K_1 > 0, \tag{3}$$

the Ising model also has a two-component order paremeter, whose components can be chosen to be the A- and B-sublattice antiferromagnetic staggered magnetizations.

Using the MCRG and van Leeuwen's[8] cell-spin transformation, we have computed the continuous variation of the critical index ν upon K_4 for the Baxter model (Fig. 1) and upon $K_1/|K_2|$ for the Ising model when (3) is satisfied (see Fig. 2). The calculated values of ν are consistent with exact results[12] for the Baxter model, and with the approximate renormalization-group analysis of Nightingale[13] for the Ising model. We feel that the MCRG is more easily applicable to three and even four dimensions than the approach used by Nightingale, which is based upon calculating the correlation length of a finite strip with use of the transfer-matrix formalism. In particular, it would be very interesting to study the Ising model with nn and nnn interactions on an fcc lattice. Phani *et al.*[14] have recently considered the case of antiferromagnetic nn and ferromagnetic nnn interactions ($n=3$-component order parameter) with use of a Monte Carlo analysis. Further insight may be gained by extending their work using the MCRG. The case of ferromagnetic nn and antiferromagnetic nnn interactions exhibiting type-II antiferromagnetic order ($n=4$-component order paremeter) has been predicted to exhibit a first-order transition on the basis of the absence of a stable fixed point in the ϵ expansion.[15] However, the type-II antiferromagnets CeSe and CeTe have been found to exhibit a continuous transition,[16] and so calculations directly in three dimensions are clearly desired.

In addition to determining ν, we have found $\eta=\frac{1}{4}$ independent of the interaction parameters for both the Baxter model and the Ising antiferromagnet, in agreement with what is expected on the basis of scaling theories.[17] We have also computed the crossover exponent y_s corresponding to nearest-neighbor exchange in the Baxter model, and the anisotropic nearest-neighbor exchange in the Ising antiferromagnet. In the limit when the A and B sublattices are decoupled, we find agreement with van Leeuwen's[8] result, and our calculation shows that the crossover exponent y_s varies with the interaction parameters in both the Baxter and Ising models (see Figs. 1 and 2).

The MCRG calculation[3,4] is based upon a MC simulation to obtain a sequence of configurations from which the necessary correlation functions can be computed. The RG transformation is then

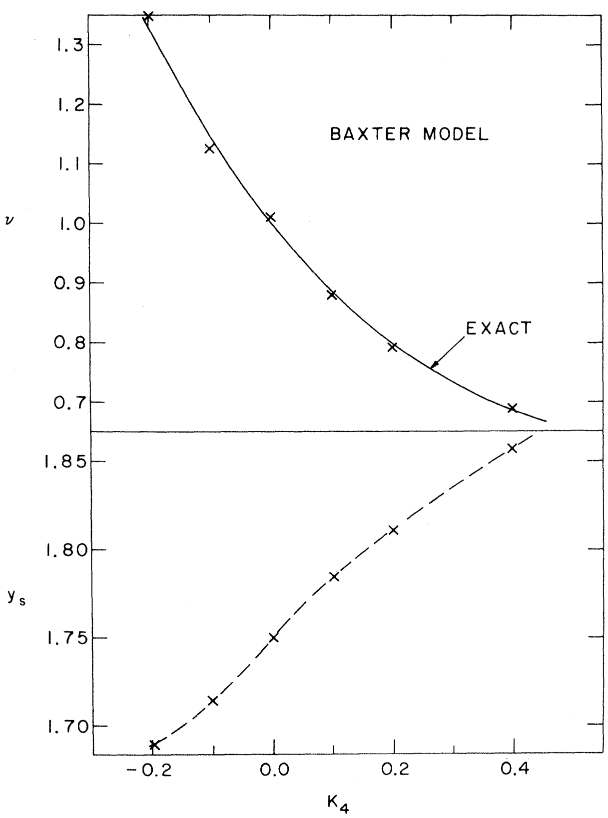

FIG. 1. ν and y_s vs K_4 for the Baxter model. Solid line indicates the exact (Ref. 12) values of ν.

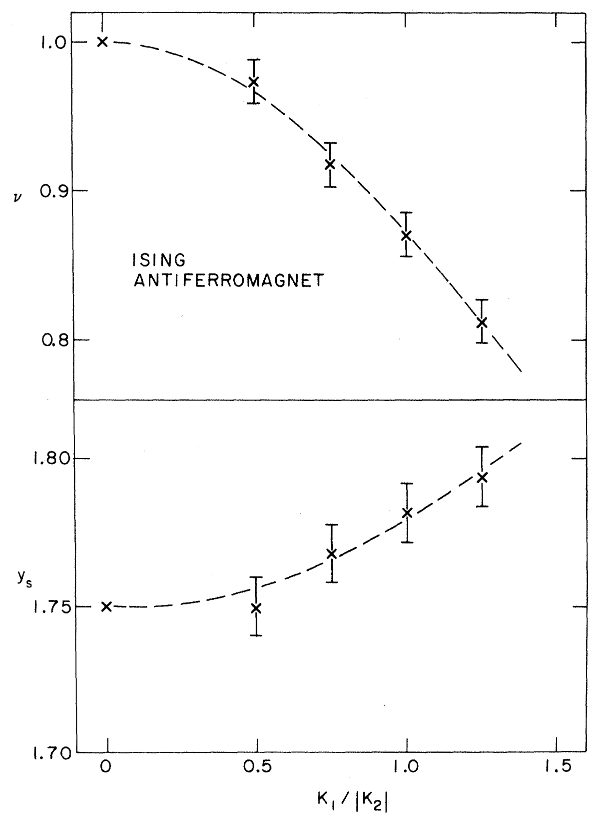

FIG. 2. ν and y_s vs $(K_1/|K_2|)$ for the Ising antiferromagnet.

applied directly to the individual configurations, yielding a sequence of configurations for the cell spins. For the Baxter model we use van Leeuwen's[8] RG transformation, obtained by dividing the square lattice into cells consisting of a central spin and its four next-nearest neighbors, as shown in Fig. 1 of Ref. 8, and assigning the value of the cell spin $S_i = \pm 1$ according to the majority rule. For the Ising antiferromagnet, the only change in the RG transformation is to give the central spin a weight of -1. The five spins in a given cell all belong to the same sublattice, A or B, and hence the two components of the order parameter are treated separately. The scale factor is $b = \sqrt{5}$ and the eigenvalues of the RG transformation have the form $\lambda = b^y$, where y is called the eigenvalue exponent. We adopt van Leeuwen's[8] notation for these exponents: The crossover exponent is y_s, corresponding to nearest-neighbor exchange in the Baxter model and anisotropic nearest-neighbor exchange in the Ising antiferromagnet; the thermal exponent is $y_T = \nu^{-1}$; the magnetic exponent is $y_H = (d+2-\eta)/2$; y_M corresponds to three-spin interactions and y_B to the direction along the Baxter fixed line.

Van Leeuwen[8] was able to determine the exact values of these exponents in the limit of decoupled A and B sublattices, by relating them to the exponents of the Ising model with only nearest-neighbor interactions. In the decoupling limit the MCRG yields results in excellent agreement with the exact values for y_s, y_T, y_H, and y_M. For nonzero interactions between the sublattices the MCRG seems well behaved and convergent to a fixed point. Although our calculation is not good enough to determine the marginal exponent $y_B = 0$, we do find the variation of the critical exponents with the strength of the interaction coupling the sublattices. Hence, we do find a line of fixed points, but we are unable to calculate the corresponding marginal eigenvalue of the linearized transformation. For the Baxter model, we have found that a good approximation to the even eigenvalues is obtained by considering only matrix elements involving nearest-neighbor, next-nearest neighbor, and four-spin interactions. For the odd eigenvalues, the applied field and a three-spin interaction were sufficient. The inclusion of four extra even and three extra odd interactions did not lead to improvement, but appeared to make the calculation more sensitive to finite-size effects. The above remarks hold for the Ising antiferromagnet, except that to obtain the crossover exponent y_S it was necessary to include the anisotropic nearest-neighbor interaction in the analysis of the linearized RG transformation matrix.

The MCRG analysis of the Baxter model is simplified by the fact that T_c is known exactly,[10] which allows the exponents to be determined from a single MC simulation. In contrast, it was necessary to determine T_c for the Ising antiferromagnet by watching the RG flows.[3,4] For temperatures about 1% above or below T_c, one clearly sees the iteration towards high- or low-temperature fixed points. To obtain greater accuracy we chose T_c to optimize convergence of the exponents. This procedure determined T_c to about 0.2%, which is better than one is able to do with conventional MC methods[18] or series expansions[19] for this model. However, the remaining uncertainty in T_c introduces a corresponding uncertainty in the exponents of the Ising antiferromagnet, which is absent in the MCRG analysis of the Baxter model. Our results for the critical coupling can be parametrized as

$$-K_{2c} = 0.440\,687 + (0.0312 \pm 0.0010)(K_1/K_2)^2 + (0.0084 \pm 0.0010)(K_1/K_2)^4. \tag{4}$$

As an illustration of the convergence of our results, we present in Table I MCRG data for a Baxter model ($K_2 = 0.314\,091$, $K_4 = 0.2$) and an Ising antiferromagnet ($K_1 = 0.6375$, $K_2 = -0.510$). For the Baxter model, the MC simulation was performed on a 100×100 lattice with periodic boundary conditions averaged over 3×10^4 MC steps/site after discarding 4×10^3 MC steps/site. For the Ising antiferromagnet, the MC simulation was on a 100×100 lattice with periodic boundary conditions averaged over 2×10^4 MC steps/site after discarding 3×10^3 MC steps/site.

The examples presented in Table I were chosen because they appear to converge to very nearly the same fixed point, as seen by a comparison of the eigenvalue exponents. In both the Baxter model and the Ising antiferromagnet, y_H remains at its Ising value of 1.875, and within the accuracy of the calculation y_M is indistinguishable from its value in the decoupled limit of 0.875. The variation of y_s and ν with the coupling between sublattices is shown in Figs. 1 and 2. The values of ν in the Baxter model agree with the exact results[12] also shown, and the values of ν for the Ising antiferromagnet are consistent with Nightingale's[13] approximate calculation. We be-

TABLE I. Two examples illustrating the convergence of the MCRG.

		BAXTER MODEL					ISING ANTIFERROMAGNET				
RG Iteration	Number of Couplings	y_S	$y_{T(=\nu^{-1})}$	y_B	y_H	y_M	y_S	$y_{T(=\nu^{-1})}$	y_B	y_H	y_M
1	1	1.7997	-	-	1.8601	-	1.7684	1.203	-	1.8485	-
	2	1.7999	1.220	-	1.8628	.645	1.7685	1.138	-.51	1.8463	.658
	3	1.7999	1.181	-.56	1.8622	.682	1.7685	1.142	-.51	1.8453	.725
	4	1.7999	1.203	-.55	1.8624	.738	1.7685	1.143	-.51	1.8442	.761
	5	1.7999	1.203	-.55	1.8622	.750	1.7684	1.146	-.51	1.8428	.761
2	1	1.8014	-	-	1.8659	-	1.7955	1.224	-	1.8723	-
	2	1.8011	1.256	-	1.8666	.808	1.7953	1.231	-.67	1.8665	.860
	3	1.8011	1.250	-.63	1.8667	.830	1.7950	1.244	-.75	1.8665	.886
	4	1.8011	1.257	-.65	1.8667	.849	1.7951	1.243	-.75	1.8666	.894
	5	1.8011	1.256	-.67	1.8659	.865	1.7951	1.241	-.75	1.8668	.882
3	1	1.8047	-	-	1.8677	-	1.7932	1.253	-	1.8785	-
	2	1.8053	1.260	-	1.8711	.837	1.7945	1.231	-.48	1.8701	.870
	3	1.8053	1.252	-.58	1.8713	.877	1.7938	1.241	-.51	1.8701	.908
	4	1.8053	1.274	-.58	1.8711	.892	1.7939	1.238	-.51	1.8701	.923
	5	1.8056	1.271	-.58	1.8700	.908	1.7940	1.229	-.53	1.8702	.919
Exact			1.248	0	1.8750						

lieve that the results reported here suggest that it will be fruitful to apply the MCRG to other Ising models with $n \geq 2$. The nature of the phase transitions in many such models is at present unknown, but of great interest.

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Note added.—Our results are in excellent agreement with the scaling relation[20] $y_s = \frac{3}{2} + \frac{1}{4} y_T$.

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