New Universal Behavior for the Impure Baxter Model

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We have extended the Monte Carlo renormalization-group method to study the isotropic Baxter model with random, quenched, site impurities. The results suggest that the critical behavior can be characterized by the pure Baxter fixed line for negative four-spin coupling terminating at the Ising fixed point.

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The effects of quenched impurities on the critical behavior of magnetic systems in two dimensions have received considerable attention in recent years.[1–13] One prediction of impurity effects comes from the Harris conjecture[1] which states that if random, quenched impurities are added to a magnetic system, new critical exponents are found only when α is positive. Renormalization-group (RG) studies of an m-component continuous-spin model with random, quenched impurities[2–7] have also shown that if the original system has a positive α a new "random" fixed point is stable and the exponents then change. Exact work[8] on a rectangular Ising model with quenched, point defects has demonstrated that the critical temperature, but not the critical exponents, depend on impurity concentration. Monte Carlo (MC) simulations for two-dimensional Ising models,[9–11] where $\alpha = 0$ in the pure models, with quenched, site impurities have also found no evidence for changes in critical-exponent behavior. However, studies[12,13] of the impure Baxter-Wu model, where $\alpha = \frac{2}{3}$ in the pure system, show that new critical behavior is indeed seen after quenched, site impurities are added to the system.

In this Letter, we will consider the effects of random, quenched, nonmagnetic, site impurities on the critical behavior of the symmetric eight-vertex (or Baxter) model.[14] This model,[15] which is exactly soluble in the absence of impurities, involves a two- and a four-spin interaction, and is unique in that several of its critical exponents vary continuously with the strength of the four-spin interaction. Since the specific-heat exponent α for the pure system can be varied continuously, we can use this model to test the Harris conjecture.[1] While this conjecture predicts qualitative changes in exponent behavior, it does not predict the new values of the exponents. Our study will provide quantitative estimates for the exponents of the impure Baxter model.

Harris has also predicted that for positive α, new behavior will only be seen within a critical region of temperature about $T_c(x)$ on the order of $x^{1/\alpha}$, where x is the fraction of quenched, nonmagnetic impurities present in the system. Monte Carlo studies of the simple-cubic Ising model[16] ($\alpha \simeq 0.12$) have not observed any changes in critical exponents with the addition of quenched, site impurities, but the predicted width of the impure critical region is probably too narrow to see any new behavior. This possibility must be considered in the present analysis for critical regions which are predicted to be small.

To determine the impure Baxter exponents, we use the Monte Carlo renormalization-group (MCRG) method[17] which has been quite successful[18] in reproducing the critical exponents of the pure Baxter model. Since this method requires accurate estimates of the critical temperature, we also employ the MCRG method[19] to determine T_c.

The Hamiltonian of the Baxter model is given by ($K_2 > 0$)[20]

$$\mathscr{H} = -K_2 \sum_{\mathrm{nnn}} \sigma_i \sigma_j - K_4 \sum_{\langle ijkl \rangle} \sigma_i \sigma_j \sigma_k \sigma_l, \qquad (1)$$

where a factor of $1/kT$ has been absorbed in the K_i. The first summation is over next-nearest neighbors (nnn) and the second is over the vertices of a nearest-neighbor (nn) square; the spins take on the values $\sigma_i = \pm 1$ and the nonmagnetic impurities, which are randomly quenched in the lattice, are represented by $\sigma_i = 0$. Monte Carlo simulations are performed on $L \times L$ lattices with several impurity quenchings and the data are averaged in the analysis. Multiple quenchings are essential to represent adequately the various possible distributions of impurities, with larger numbers of quenchings needed as the lattice size decreases.

In the MCRG approach, the RG transformation is applied directly to the spin configurations generated by the MC simulation, producing configurations for the renormalized spins. These new renormalized spin configurations allow us to calculate any correlation functions of interest corresponding to the effective renormalized Hamiltonian.

To extend the MCRG method to include quenched impurities, a full treatment would involve an independent renormalization of the quenched variables. However, for the questions we are interested in, we have chosen a simplified representation in which only the spin variables appear explicitly in the RG transformation. Spins are assigned to all sites, but spins on vacancies are assigned ± 1 with equal probability. The presence of a quenched vacancy is then represented by a spin that has zero correlations with the rest of the lattice. Applying a majority-rule transformation with five-spin blocks allows the system to renormalize to a fixed point with or without residual quenched impurities.

Critical exponents are obtained from the eigenvalues of the matrix

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

where $K_\alpha^{(n)}$ is the coupling constant corresponding to the operator $S_\alpha^{(n)}$ on the nth RG transformation. $T_{\alpha\beta}$ is found from the chain-rule equation

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

where the square brackets indicate the average over the quenched variables and

$$\frac{\partial[\langle S_\gamma^{(n)}\rangle]}{\partial K_\beta^{(n-1)}} = [\langle S_\gamma^{(n)} S_\beta^{(n-1)}\rangle - \langle S_\gamma^{(n)}\rangle\langle S_\beta^{(n-1)}\rangle]. \tag{4}$$

Before applying the MCRG technique outlined above, we need to accurately determine the critical temperature T_c. Therefore, we locate T_c by carrying out MC simulations on two different lattices which differ in linear dimension by the RG scale factor b.[19] By applying an RG transformation to the larger lattice, we then have two lattices of the same size; the differences in the correlation functions of these lattices correspond to differences between the original and renormalized Hamiltonians. Changes in the coupling constants of the original Hamiltonian needed to make the correlation functions equal are determined by solving the equation

$$[\langle S_\alpha^{(n)}\rangle]_L - [\langle S_\alpha^{(n-1)}\rangle]_S = \sum_\beta \left(\frac{\partial[\langle S_\alpha^{(n)}]_L}{\partial K_\beta^{(0)}} - \frac{\partial[\langle S_\alpha^{(n-1)}\rangle]_S}{\partial K_\beta^{(0)}} \right) \delta K_\beta^{(0)}, \tag{5}$$

where the subscripts L and S refer to the "large" and "small" lattices. The derivatives are calculated as in Eq. (4). This procedure becomes more sensitive to relevant perturbations (and insensitive to irrelevant ones) as n increases. Since the original Baxter Hamiltonian involves two couplings, we fix the four-spin coupling K_4 and vary the two-spin coupling K_2 on the basis of the changes predicted by Eq. (5). Table I illustrates the predicted changes in the two-spin coupling K_2 for one negative and two positive values of K_4 with $x = 0.125$. Predictions are shown for several values of K_2 in the vicinity of the critical coupling K_{2c}. As can be seen, these predictions for K_2, both above and below K_{2c}, point back to the critical value of K_2.

Once T_c has been accurately determined, the MCRG method is used to estimate the critical exponents. Details of MCRG runs are given in Table II, and Table III shows the exponent estimates from the successive RG iterations for each of three values of K_4, along with the corresponding pure ex-

TABLE I. Predicted change in two-spin coupling $\delta K_2^{(0)}$ with $L = 20\sqrt{5}$ for the large lattice and $L = 20$ for the small lattice. The numbers of MC steps/spin and quenchings used are 1.5×10^4 MC steps/spin and $Q = 15$ for $L = 20\sqrt{5}$ and 8×10^3 MC steps/spin and $Q = 40$ for $L = 20$.

$\alpha = -0.520$ $K_4 = -0.200$			$\alpha = 0.372$ $K_4 = 0.240$			$\alpha = 0.491$ $K_4 = 0.360$		
K_2	$\delta K_2^{(0)}$	$K_2 - \delta K_2^{(0)}$	K_2	$\delta K_2^{(0)}$	$K_2 - \delta K_2^{(0)}$	K_2	$\delta K_2^{(0)}$	$K_2 - \delta K_2^{(0)}$
0.6826	−0.0026	0.6852	0.3726	−0.0031	0.3757	0.4162	−0.0058	0.4220
0.6862	0.0033	0.6829	0.3752	−0.0004	0.3756	0.4240	−0.0001	0.4241
0.6891	0.0023	0.6868	0.3779	0.0025	0.3754	0.4272	0.00005	0.42715

TABLE II. Data for MCRG calculations in Table III.

	Number of MC steps/spin per quenching	Number of quenchings
$L=20$, all cases	8.0×10^3	40
$L=20\sqrt{5}$, all cases	1.5×10^4	15
$L=100$		
$K_4=-0.2$	5.0×10^4	6
$K_4=0.24$	6.0×10^4	6
$K_4=0.36$	6.0×10^4	6

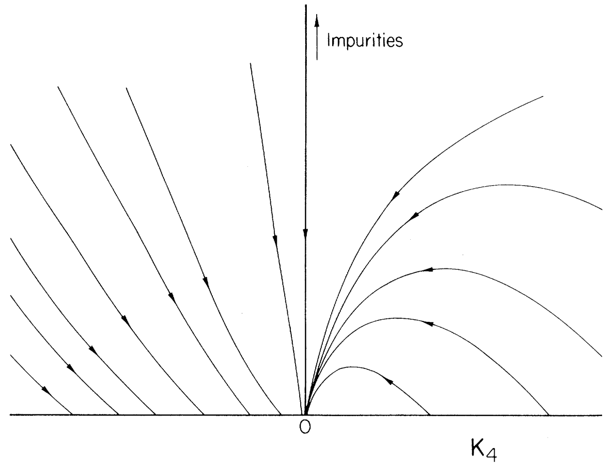

FIG. 1. Schematic renormalization flow diagram.

ponents. The exponents listed are average values obtained from the analyses that use the three or four largest numbers of couplings. For $K_4=-0.2$ ($\alpha=-0.52$ for the pure lattice) we find convergence to the pure Baxter exponents. The convergence, when compared with previous results,[18] has been slowed down by the addition of impurities, which indicates that the impure fixed point is farther away than the corresponding pure one. Finite-size effects are evident in the last iteration, which corresponds to a 4×4 lattice.

Exponent flows for both values of $K_4>0$ demonstrate that these impure critical exponents are markedly different from pure exponent values! Differences are quite evident in the thermal exponent y_T and the crossover exponent y_S. For $K_4=0.24$ ($\alpha=0.372$ for the pure lattice) we obtain $y_T=0.97\pm0.07$ ($\nu=1.03\pm0.08$) and $y_S=1.75\pm0.05$, which compare with the exact values of $y_T=1.228$ and $y_S=1.807$ for the pure model. For $K_4=0.36$ ($\alpha=0.491$ for the pure lattice) we get $y_T=0.98\pm0.07$ and $y_S=1.77\pm0.04$, and the corresponding pure exponent values are $y_T=1.325$ and $y_S=1.831$. The exponents do not converge as well as for the negative-K_4 ($\alpha<0$ for the pure lattice) case, which is understandable since Harris predicts that new critical behavior will be seen only in a critical region in width $x^{1/\alpha}$. For $x=0.125$ and

TABLE III. Eigenvalue exponent variation with iteration for impurity concentration $x=0.125$.

		$K_{4C}=-0.200$		$K_{2C}=0.6862$		$K_{4C}=0.2400$		$K_{2C}=0.4240$		$K_{4C}=0.3600$		$K_{2C}=0.3752$	
	Iteration	Y_S	Y_T	Y_H	Y_M	Y_S	Y_T	Y_H	Y_M	Y_S	Y_T	Y_H	Y_M
L=20	1	1.480	0.32	1.784	0.37	1.580	0.57	1.759	0.16	1.609	0.58	1.760	0.02
	2	1.664	0.78	1.860	0.79	1.717	0.95	1.841	0.71	1.732	0.97	1.846	0.66
$L=20\sqrt{5}$	1	1.482	0.270	1.783	0.28	1.596	0.540	1.768	0.36	1.624	0.568	1.761	0.19
	2	1.662	0.74	1.857	0.69	1.737	0.92	1.847	0.70	1.754	0.95	1.846	0.64
	3	1.708	0.87	1.875	0.81	1.736	0.95	1.864	0.81	1.770	1.02	1.870	0.78
L=100	1	1.476	0.32	1.783	0.42	1.603	0.56	1.765	0.42	1.632	0.59	1.760	0.25
	2	1.658	0.74	1.856	0.76	1.742	0.90	1.845	0.71	1.768	0.93	1.849	0.67
	3	1.699	0.83	1.875	0.82	1.755	0.94	1.857	0.74	1.786	0.96	1.870	0.78
	4	1.67	0.85	1.88	0.92	1.70	0.96	1.83	0.74	1.76	1.01	1.87	0.77
	Pure	1.698	0.794	1.875	0.669	1.807	1.228	1.875	1.103	1.831	1.325	1.875	1.200
			$\alpha=-0.520$				$\alpha=0.372$				$\alpha=0.491$		

$\alpha = 0.372$ this width is $x^{1/\alpha} \sim 0.004$ as compared with $x^{1/\alpha} \sim 0.014$ for $\alpha = 0.491$ and the same x.

Our results substantiate the validity of the Harris conjecture and are consistent with the schematic RG flow diagram shown in Fig. 1. For $K_4 < 0$ ($\alpha < 0$) the impurities are irrelevant, so that the pure fixed line also describes the model with quenched impurities. The value of α could change slightly from the pure model with the same ratio of K_2/K_4, but this effect is too small for us to resolve.

For $K_4 > 0$ ($\alpha > 0$), the RG trajectories flow away from the pure Baxter fixed line and we see a large change in the value of α. Since the new critical exponents are equal to the pure Ising exponents (within statistical errors) for the $K_4 = 0.24$ and 0.36 cases, it suggests that the pure Ising fixed point ($K_4 = 0$) describes all systems with quenched vacancies and $K_4 > 0$ ($\alpha > 0$), as indicated in Fig. 1. It is interesting to note that the value of $y_T = 0.98 \pm 0.07$ which we obtain for positive K_4 compares favorably with studies of the impure Baxter-Wu model[12,13] and with impure Ising results.[9-11]

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