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Monte Carlo renormalization-group study of the site-diluted simple-cubic Ising model

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The Monte Carlo renormalization-group approach is applied to investigate the critical behavior of the simple-cubic Ising model diluted randomly with nonmagnetic atoms of concentration x. For $x=0.2$ a value of $\nu=0.688(13)$ is found which is well above the result $\nu=0.629(4)$ for the pure model and above the exact lower bound of $\nu=\frac{2}{3}$, and the relative width of the asymptotic regime is definitely larger than 3×10^{-4}. For $x=0.1$ the obtained value is below the exact lower bound, possibly indicating that the asymptotic critical regime has not been penetrated, that this regime has a width smaller than 1.3×10^{-4}, and that it can hardly be explored by experiments or computer simulations.

The critical behavior of spin systems with random structural disorder has been discussed for almost 20 years. According to the phenomenological arguments of Harris,[1] systems with weak disorder should exhibit the same critical behavior as the one of the corresponding pure system if the specific-heat exponent α_p of the pure system is negative, as in the case of $d=3$ Heisenberg ferromagnets (for a review of experimental verifications see Refs. 2 and 3). In contrast, the critical behavior is expected to be modified by disorder for $\alpha_p>0$, for instance for the $d=3$ Ising model. The latter statement has been proved rigorously by Chayes *et al.*[4] who derived an inequality for the correlation exponent ν of disordered systems, $\nu\geq 2/d$, yielding $\alpha=2-d\nu\leq 0$, which contrasts to $\nu_p=0.63$ and $\alpha_p=0.11$ for the pure $d=3$ Ising model.

Whereas the existence of a stable random Ising fixed point is thus well established, no consensus has emerged so far concerning (a) the precise values of the exponents and their possible dependences on the degree of disorder, i.e., the concentration x of nonmagnetic atoms in a site-diluted system; (b) the width of the asymptotic critical regime, which—according to Harris[1]—should depend strongly on x. Various k-space renormalization calculations[5] for weakly disordered systems obtained results for ν between 0.67 and 0.697, i.e., consistently higher than the theoretical lower bound of $\nu=\frac{2}{3}$ and independent of x, without giving any estimate for the width of the asymptotic critical regime. The results of Monte Carlo simulations (MC) are divided. Whereas the early small-system simulations were consistent[6] with a pure-fixed-point behavior, later investigations[7-10] revealed modified effective exponents which depend[7,8] on x and which are for small x so close to the pure system values that the criterion $\nu\geq\frac{2}{3}$ is violated. The most recent simulation[11] obtained impure critical exponents which did not depend on x but which differed significantly from those of the k-space renormalization calculations (e.g., $\nu=0.77\pm0.04$). Similarly, the experimental investigations were inconclusive (for a review see Refs. 9 and 10). Altogether, it may be suspected that all the inconsistencies may arise because the width of the asymptotic regime is very small and depends on x, so that part of the MC and the experimental investigations were not able to penetrate this regime or yielded at most an effective average exponent over a large temperature range.

In this paper we present a Monte Carlo renormalization-group (MCRG) study[12] for simple-cubic Ising systems with quenched random site dilution. We consider $x=0$ and the weakly diluted limit ($x=0.1$, 0.2) for which the k-space renormalization calculations most probably yield reliable results. Our aim is to try to reproduce these results by the present real-space renormalization technique, and to obtain, in addition, an estimate for the width of the asymptotic regime.

Our procedure is very much in line with the MCRG of Pawley *et al.*[13] for the pure ($x=0$) simple-cubic Ising model, and we discuss only the modifications introduced by the dilution. MC simulations based on a fully vectorized multispin coding program[8,10] have been performed for lattices with 64^3, 32^3, and 16^3 spins with 2, 4, and 8×10^6 sweeps, respectively, for $x=0.1$ as well as 2, 3, and 4×10^6 sweeps for $x=0.2$, taking the data after every fourth sweep for the thermal averaging. Two different kinds of majority rules have been applied for each concentration, one where we assign spins ±1 with equal probability to the nonmagnetic sites,[14] and one where we associate a nonmagnetic site with spin 0. Both procedures lead to consistent final results, but the latter one exhibits a faster convergence. We considered the same even correlation functions as in Ref. 13, as well as a single spin and three three-spin correlations (inclusion of higher-order odd correlations did not change the results beyond the statistical significance).

For a reliable determination of the thermal eigenvalue $y_T=1/\nu$ and the magnetic eigenvalue $y_H=(d+2-\eta)/2$ the MCRG calculation must be performed accurately at T_c. In a pure system T_c is usually obtained from the demand that all correlation functions (in practice the nearest-neighbor correlations) for lattices of different sizes but correspondingly different blocking levels n (same "effective" sizes) should be equal ("lattice comparison").

For diluted systems, however, this procedure is not reliable because there may be rather big differences in the pseudocritical temperatures for different lattice sizes due to different configurations of nonmagnetic atoms. As a re-

sult, the lattice comparison may stabilize at a temperature which is the critical temperature of neither of the considered lattices. Because the results of the MCRG depend extremely sensitively on the choice of the critical temperature, there may arise very big errors from this uncertainty. We are not certain whether the problem may be overcome by performing a configurational average for the lattices before the lattice comparison. Because the lattice sizes are smaller than the thermal correlation length, the situation is not ergodic, i.e., we cannot simulate a big lattice by a configurational average over many small lattices. Furthermore, a configurational average over many 64^3 lattices is beyond our computational capabilities.

To cope with the above-discussed problem we proceed on the following line: We consider only one lattice of size 64^3 with randomly distributed nonmagnetic atoms, but we generate many 32^3 and 16^3 lattices, each of them with different impurity configuration. For all these lattices we perform the MC simulation at, say, four different temperatures which are close to the infinite-lattice critical temperature predicted by a conventional MC simulation. We then select from this set of lattices those triplets of 64^3, 32^3, and 16^3 lattices for which the lattice comparison stabilizes at a temperature near one of these four temperatures. To cope with the above-discussed uncertainty, we carry out the following consistency check.[12,15] We perform the MCRG analysis of the 64^3 lattice at all considered temperatures on the line described in Ref. 13, being well aware of the fact that the finite-size corrections (for which we need the data of the corresponding 32^3 and 16^3 lattices) may be erroneous if the lattice comparison did not yield the correct critical temperature. If everything is reasonable we expect results for y_T vs 2^{-n} like those shown in Fig. 1 (in all our cases the largest negative eigenvalue turned out to be close to -1, which justifies the plot y_T vs 2^{-n}). For $T=T_c$ [Fig. 1(b), the noncorrected data are given in Table I] there is an indication of a plateau for large blocking levels n. For the larger temperature, Fig. 1(c) shows a situation for which after an initial approach to the fixed point the trajectory in the parameter space is clearly driven away from the fixed point. Such a behavior of y_T is typical for temperatures above T_c. Figure 1(a) demonstrates that for the lower temperature an upward bending of the curve is obtained for large n, which is typical for temperatures below T_c. Since even for the correct T_c the plateau could possibly occur only for larger than the considered values of n, we must find a further criterion for a lower limit of T_c. We assume that the considered temperature is certainly below the correct T_c if the energy per spin is already larger than the energy per spin of the pure model at the critical temperature of the pure model. Although apart from the diluted honeycomb lattice[16] there is no general proof for this assumption, it seems to be highly reasonable. Altogether, the behavior of y_T vs 2^{-n} for different temperatures as shown in Fig. 1 suggests that the lattice comparison yielded the correct critical temperature. For other triplets of lattices we can find situations for which at the "critical temperature" of the lattice comparison a behavior such as in Fig. 1(a) with a violation of our energy criterion occurs, indicating that the obtained critical temperature is too low. Alternatively, we can also find situations for which at the critical temperature Fig. 1(c) holds, indicating a too high temperature. All these pathological situations are eliminated.

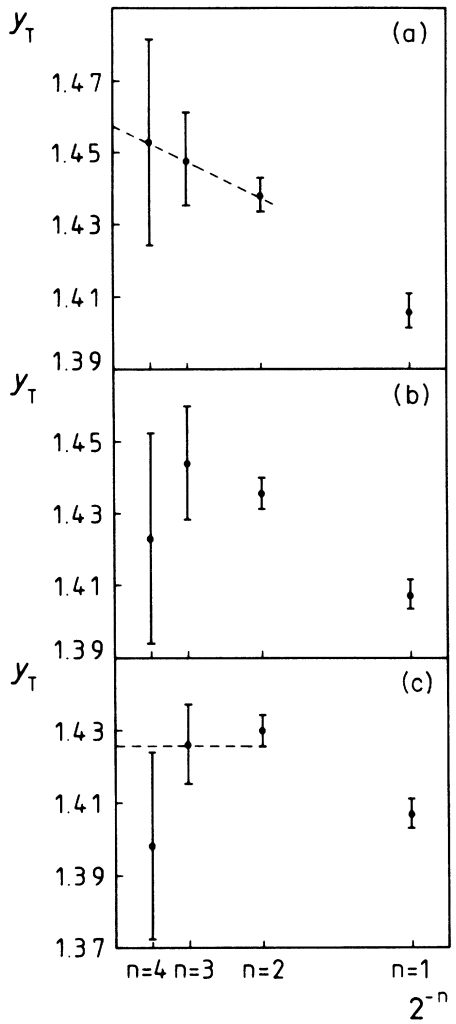

FIG. 1. Estimates for $1/\nu$ at (a) $1/K_1=3.4980$, (b) 3.4985, and (c) 3.4990, plotted vs 2^{-n}. The dashed line in (a) indicates the linear fit to the data points for $n=2$, 3, and 4 yielding an extrapolated value of $y_T=1.4584(224)$ with an upper limit of $y_T=1.4808$. The dashed line in (c) represents the lower limit for y_T.

The above-discussed procedure is able to enclose the critical temperature of a triplet in an interval which is, for $x=0.2$, an order of magnitude smaller than the spread in the critical temperatures of all our 32^3 lattices and hence—according to simple statistical assumptions—a factor of 3 smaller than the spread for the 64^3 lattice.

The final result for y_T is found in the following way: We first extrapolate the last three points ($n=2,3,4$) in Fig. 1(a) linearly in 2^{-n} as in Ref. 13, yielding for $x=0.2$ an estimate $y_T=1.4584(224)$ and an upper limit of $y_T=1.4808$. To obtain a lower limit we note again that the correct critical temperature is somewhere between cases 1(a) and 1(c), and that we expect a plateau for large n at this temperature. Assuming that the approach to this plateau is monotonic, we obtain a lower limit of y_T

TABLE I. The MCRG table in the form of Ref. 13 for the thermal eigenvalue $y_T = 1/\nu$ for $x = 0.2$ and $1/K_1 = 3.4985$. Because the results of the first renormalization step have only a negligibly small effect on the final exponent values, we have calculated the correlation functions for the original lattice with poorer statistics, thereby saving about $\frac{2}{3}$ of the computer time.

64	32	16
0.8343	0.8388	0.8298
0.9144	0.9227	0.9179
0.9139	0.9226	0.9178
0.9121	0.9209	0.9139
0.9099	0.9184	0.9120
0.9003	0.9075	0.9018
0.8979	0.9054	0.8975
1.3705(10)	1.3609(11)	1.3527(10)
1.4148(11)	1.4099(12)	1.4157(12)
1.4148(11)	1.4100(13)	1.4162(13)
1.4144(11)	1.4091(13)	1.4135(13)
1.4139(11)	1.4078(14)	1.4126(12)
1.4121(12)	1.4058(14)	1.4104(14)
1.4074(12)	1.3994(15)	1.4012(15)
1.4063(21)	1.4234(21)	1.5439(23)
1.4484(21)	1.4796(22)	1.6457(23)
1.4476(23)	1.4795(27)	1.6519(23)
1.4467(23)	1.4739(28)	1.6342(25)
1.4456(22)	1.4712(28)	1.6298(24)
1.4431(22)	1.4678(29)	1.6236(25)
1.4357(22)	1.4594(30)	
1.4301(33)	1.5854(52)	
1.4827(32)	1.6839(52)	
1.4813(34)	1.6915(51)	
1.4769(33)	1.6700(50)	
1.4755(35)	1.6634(49)	
1.4724(35)	1.6565(49)	
1.4639(34)		
1.5790(82)		
1.6786(81)		
1.6861(79)		
1.6641(87)		
1.6551(77)		
1.6479(84)		

$= 1.4256$ as shown in Fig. 1(c). The assumption of a monotonic exponent flow is equivalent to the notion that the thermodynamic behavior in the considered temperature range is determined by only one fixed point, i.e., that the system is driven directly to the stable fixed point. Otherwise there could be a crossover from an unstable fixed point which determines the flow at low blocking levels to the stable asymptotic fixed point at high blocking levels (perhaps at higher than the considered ones), yielding possibly a nonmonotonic flow.

Our results are summarized in Fig. 2. For $x = 0$ we obtain the same value of ν as in Ref. 13. For $x = 0.2$ the value is above the lower limit[4] of $\nu = \frac{2}{3}$ and within the range obtained by the k-space renormalization calculations. This suggests that we have found the correct

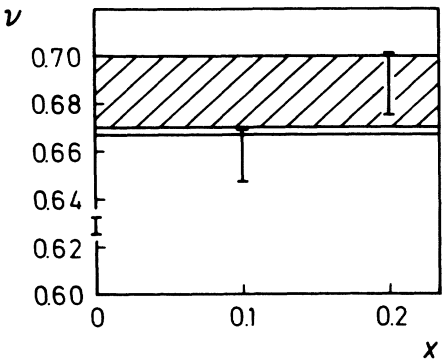

FIG. 2. Results for ν as function of x. The lower solid line indicates the exact lower bound of Ref. 4, and the shaded area indicates the range of values obtained by the k-space renormalization calculations.

asymptotic critical value and that the width $\Delta T/T_c$ of the asymptotic critical regime is at least as large as our relative uncertainty for the critical temperature (3×10^{-4}) defined by the lower and upper limits [Figs. 1(a) and 1(c)]. Furthermore, from our data we do not see the influence of any other fixed point (e.g., the pure Ising fixed point) in the lower blocking levels. For $x = 0.1$ the value of ν is below the limit of $\nu = \frac{2}{3}$, i.e., we have determined an effective rather than the asymptotic exponent. If the critical behavior is determined by only one fixed point, this result indicates that none of the three considered temperatures in the interval $\Delta T/T_c = 1.3\times10^{-4}$ was within the asymptotic critical regime, that for weakly diluted systems the width of the asymptotic critical regime is very small (according to Harris[1] proportional to x^{1/α_p}) and that it can hardly be penetrated by experimental investigations and computer simulations for finite lattices. Alternatively, it may also be possible that there are two fixed points and that for $x = 0.1$ a crossover to the asymptotic fixed point is observable only in larger systems at larger than the considered blocking levels. In this case we cannot say anything about the width of the asymptotic critical regime. However, the obtained exponent flow then would indicate that the unstable fixed point is most probably the homogeneous fixed point as discussed in Refs. 17 and 18 and not a fixed point with totally different exponent values (e.g., the random tricritical fixed point with $y_T = \nu = 1$ discussed in Ref. 19).

Because for diluted systems the error bars are considerably larger than for the pure model (cf. Fig. 1), the η values which result from the difference of two large numbers, $\eta = 5 - 2y_H$ for $d = 3$, could only be enclosed in the reasonable, albeit wide, interval $0 < \eta < 0.05$ for $x = 0.1$ and $x = 0.2$. The flow of the η values is thereby consistent with the flow of the y_T values as shown in Fig. 1, constituting a further consistency check for the critical temperature. For example, for the temperature of Fig. 1(a) the extrapolated η value is already negative, indicating that the temperature is definitely too low.

For a stronger dilution ($x = 0.4$) the statistical accuracy of our MCRG approach was too poor to obtain reliable estimates for the exponents. A very detailed description of the calculation will be given in Ref. 20.

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