

## Monte Carlo simulation of strongly disordered Ising ferromagnets

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We report extensive Monte Carlo simulations of disordered Ising systems in the ferromagnetic region with concentrations of magnetic sites between  $p=1.0$  and  $0.5$ . The magnetization, the susceptibility, and the caloric properties have been studied in the critical region. The critical exponents  $\beta$  and  $\gamma$  as well as the universal amplitude  $A$  of the magnetization and the ratio  $C_+/C_-$  of the susceptibility amplitudes have been determined with high precision. In addition to the cusplike specific heat, we have also measured the magnetization-energy correlation function  $\Gamma$ , which is a *divergent* thermal quantity. The corresponding critical exponent  $\zeta$ , which is related to the other exponents by  $\zeta=1-\beta=(\alpha+\gamma)/2$ , has been determined. We have found that all quantities show power-law behavior within the temperature range of our simulation. All critical exponents change continuously with dilution. Even in the range of weak dilution ( $p \geq 0.8$ ), the effective critical exponents are concentration dependent and are clearly different from their pure system values. In the strongly diluted regime the critical exponents gradually reach new asymptotic behavior at  $p=0.5-0.6$  with values of  $\beta=0.335 \pm 0.01$  and  $\gamma=1.49 \pm 0.02$ . The exponent  $\alpha$  of the specific heat becomes  $-0.17 \pm 0.04$ , which corresponds to a cusplike singularity. We conclude that disorder profoundly changes the critical behavior for weakly as well as strongly disordered spin systems.

### I. INTRODUCTION

Critical phenomena in disordered systems have been studied for twenty years using various analytical and computational methods. However, the influence of disorder in systems with large fluctuations is still a field of active research. With considerable efforts the problem has been attacked in two extreme cases, i.e., in the limit of weak disorder<sup>1-5</sup> and near the percolation point<sup>7-11</sup> (Fig. 1). The most important conjecture concerning the criti-

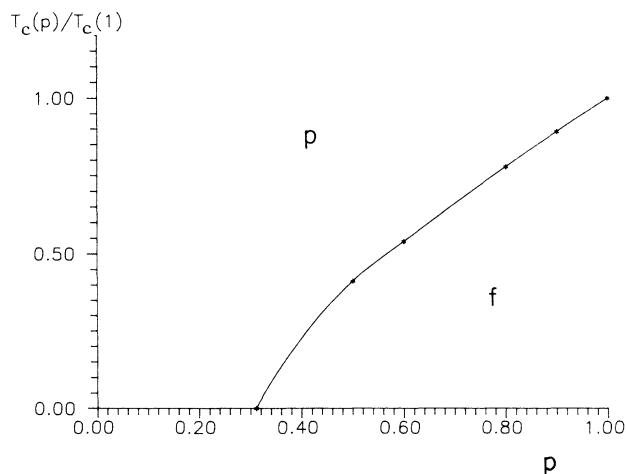


FIG. 1. Phase diagram of the site-disordered three-dimensional Ising system. The system orders ferromagnetically at the  $T_c(p)$  line; below the percolation concentration  $p_c=0.31$  ferromagnetic order is not possible. The stars indicate the concentrations  $0.5 \leq p \leq 1.0$  and respective  $T_c(p)/T(1)$  values of our simulation.

cal behavior of *weakly* disordered ferromagnets is the Harris criterion,<sup>1</sup> which states that the critical behavior remains unchanged if the exponent  $\alpha_h$  of the pure system is negative; for positive  $\alpha_h$  a new type of critical behavior should appear. Renormalization group works on weakly diluted systems<sup>2-5</sup> treat disorder as a perturbation of the pure system. They have confirmed this expectation: a new stable fixed point with new exponents appears in the case of Ising systems that have a positive critical exponent  $\alpha_h$ ; the new exponents should be independent of the concentration. In the case of Heisenberg magnets that have a negative  $\alpha_h$  the fixed point of the pure system remains stable and the critical exponents remain unchanged. To be precise, the Harris criterion is a conjecture about the asymptotic critical behavior very near  $T_c$  of *weakly* disordered systems. The crossover exponent  $\phi_x$  of disorder in the Ising model is equal to the critical exponent of the specific heat  $\alpha_h$ , which is very small [ $\alpha_h=0.11$  (Ref. 6)] so that the critical behavior of Ising systems should be modified by disorder only in remote temperature ranges such as  $|t| \leq (1-p)^{1/\phi_x}$ , i.e.,  $|t| \leq 10^{-9}$  for  $p=0.8$  ( $t=(T-T_c)/T_c$ ). Thus, experiments with real ferromagnets as well as simulations of spin systems in the temperature range  $10^{-3} \leq |t| \leq 10^{-1}$  around the critical temperature  $T_c$  should not detect a change of the critical exponents by disorder. However, there is no quantitative measure of what *weakly* disordered actually means, i.e., in which range of dilution and temperature the perturbative approaches<sup>1-5</sup> and their results are applicable.

Other works on critical behavior in disordered systems have started from strongly disordered systems, i.e., from the percolation threshold<sup>7-10</sup> which can be viewed as a multicritical point (Fig. 1). The starting point of these

works is the ramified cluster structure on which quasi-one-dimensional correlations are assumed to determine the critical behavior near the critical temperature  $T_c = 0$ . It has been argued that this picture is simplified; the backbone of the percolation cluster is finitely ramified but not quasi-one-dimensional. The degree of ramification has been shown to be essential for critical phenomena.<sup>11</sup>

The purpose of this work is twofold. Simulations in the range of weak dilution should clarify in which concentration range of diluted magnets the perturbative approaches<sup>1-5</sup> to the problem are reliable and give results that are in accord with experiments. Previous attempts to study weakly diluted systems by simulations<sup>13,14</sup> have indicated a change of the critical exponent  $\beta$  upon dilution. We want to extend these works, determine the other critical exponents as well, and check whether disordered spin systems show scaling behavior at all. Our second point is the investigation of the critical behavior of strongly disordered systems. There are no quantitative results from simulations about these systems. Particularly interesting is the question whether a crossover to percolative behavior can be detected and whether the effective critical exponents are temperature and/or concentration dependent.

## II. THE METHOD

To answer these questions we have performed extensive Monte Carlo simulations<sup>15</sup> of the site-diluted Ising model in three dimensions. This model is defined by

$$H = -J \sum_{ij} K_i S_i K_j S_j, \quad (1)$$

where  $S_i, S_j = \pm 1$  are the spin variables. The summation runs over  $N = L^3$  sites of the lattice. The occupation variables are  $K_i = 1$  if a magnetic ion is at site  $i$  and  $K_i = 0$  if a nonmagnetic ion is at site  $i$ . The  $K_i$  are identically distributed with the concentration  $p$ .  $J > 0$  is the ferromagnetic nearest-neighbor coupling; the temperature will be given below in units of  $J/k$  ( $k$  being Boltzmann's constant). This model is the simplest physical system where the influence of disorder on the critical behavior can be studied. Moreover, it is the only system where a change of the critical behavior is expected at all in the region of *weak* disorder.<sup>1-5</sup>

Simulations of disordered spin systems have been relatively sparse in the past since the relaxation times increase drastically with dilution so that enormous simulation times are necessary to obtain data with sufficient accuracy to determine critical exponents. Early studies of the site-diluted Ising model (1) have been performed in 1980 by Landau<sup>12</sup> who has simulated diluted Ising systems in the concentration range  $0.2 \leq p \leq 1.0$ . He has studied system sizes up to  $30^3$  simulating 500–5000 MCS (Monte Carlo steps per spin) for each data point. Due to insufficient accuracy Landau concluded that the data were consistent with pure system exponents as theoretically expected. Further numerical work was not performed until 1986 when Marro, Labarta, and Tejada<sup>13</sup> simulated diluted Ising systems ( $p \geq 0.8$ ) with dimensions  $30^3$  and  $40^3$ . Chowdhury and Stauffer<sup>14</sup> extended their

work to a system size of  $90^3$ . These studies were performed in the *weak* dilution regime  $0.8 \leq p \leq 1.0$ . With an accuracy of 5000–10000 MCS per data point both studies detected a significant concentration-dependent increase of the effective critical exponent  $\beta$ . The critical exponent  $\gamma$  seemed to increase too, but the data for the susceptibility were not good enough for a quantitative estimate.

We have performed simulations with a system size of  $60^3$  using the standard Monte Carlo technique<sup>15</sup> with local spin dynamics. Smaller lattices were also simulated in order to study finite-size effects.<sup>16,17</sup> The concentrations range from the weak dilution regime  $p=1.0$ ,  $p=0.9$  over  $p=0.8$  to the strongly diluted systems with  $p=0.6$  and  $p=0.5$ . In order to study the configuration dependence of the results and to obtain a reasonable approximation of the thermodynamic limit, we simulated up to ten different configurations for each concentration. The systems were simulated in the critical region  $5 \times 10^{-3} \leq |t| \leq 10^{-1}$  where  $t = (T - T_c)/T_c$  and  $T_c$  is the critical temperature of the diluted system. We have performed simulations at about 40 temperatures above and below  $T_c$  in order to have a dense sequence of measurements in the critical region.

We have measured the magnetization, the susceptibility, the energy, and the specific heat. Using the abbreviation

$$M = \sum_i K_i S_i, \quad (2)$$

the spontaneous magnetization  $m$  is given by the expectation value of the absolute value of  $M$  normalized to the number of occupied sites  $pN^3$ :

$$m = \frac{1}{pN^3} \langle |M| \rangle. \quad (3)$$

The susceptibility is defined by the fluctuation of the spontaneous magnetization

$$\chi = \frac{1}{NpT} (\langle M^2 \rangle - \langle |M| \rangle^2) \quad (4)$$

below  $T_c$  and by

$$\chi = \frac{1}{NpT} \langle M^2 \rangle \quad (5)$$

above  $T_c$ .<sup>17</sup> The energy is given by

$$E = \frac{1}{Np} \langle H \rangle \quad (6)$$

and the specific heat is defined by the fluctuation

$$C = \frac{1}{NpT^2} (\langle H^2 \rangle - \langle H \rangle^2). \quad (7)$$

In Eqs. (3)–(7) the average  $\langle \rangle$  is the time average of the corresponding quantity over the whole Monte Carlo sequence after relaxation into thermodynamic equilibrium.

Previous simulations<sup>12,13</sup> have shown that the specific heat is cusplike. Therefore it is not well suited to determine the critical exponent  $\alpha$ . Even in the pure case it is difficult to extract quantitative results from specific-heat

measurements since  $\alpha$  is usually very small and the singular behavior may be masked by corrections to scaling and nonsingular terms. We therefore introduced the magnetization-energy correlation  $\Gamma$  to obtain information about the thermal critical behavior.  $\Gamma$  is defined by

$$\Gamma = \frac{\partial^2 F}{\partial H \partial t} \quad (8)$$

and is measured below  $T_c$  in our Monte Carlo simulation by the fluctuation expression

$$\Gamma = \frac{1}{NpT^2} [\langle (|M| - \langle |M| \rangle)(H - \langle H \rangle) \rangle]. \quad (9)$$

Unfortunately, as an odd power of  $M$ ,  $\Gamma$  vanishes above  $T_c$ ; its time average in a Monte Carlo simulation is then arbitrary. From the scaling behavior of the free energy

$$F(t, h) = b^{-d} F(b^{y_t} t, b^{y_h} h), \quad (10)$$

$\Gamma$  is shown to diverge as  $t^{-\zeta}$  where the exponent  $\zeta$  is given by

$$\zeta = \frac{d - y_t - y_h}{y_t} \quad (11)$$

and  $y_t$  and  $y_h$  are the exponents of the temperature and the magnetic field. From (11) and the corresponding expressions for  $\alpha$ ,  $\beta$  and  $\gamma$ , one obtains the exponent relations

$$\zeta = 1 - \beta = (\alpha + \gamma) / 2. \quad (12)$$

Since  $\Gamma$  is diverging at the critical point, it should provide a way to determine even negative exponents  $\alpha$  if  $\gamma$  and  $\zeta$  are known. Clearly, the Rushbrooke relation  $\alpha + 2\beta + \gamma = 2$  would suffice to obtain  $\alpha$  from measurements of  $\beta$  and  $\gamma$ . However, this would assume that the system shows scaling behavior. With the two-exponent relation (12) one may check whether scaling is valid at all in the temperature range where measurements have been performed. Clearly, the exponent relation (12) applies only if corrections to scaling vanish in *all* the quantities involved.

Before starting long simulation runs we have studied the relaxational behavior at various concentrations and temperatures. To this end we monitored the initial time development of the magnetization and the energy. Figure 2 shows the first 30 000 Monte Carlo updates of  $60^3$  lattices with concentrations  $p=1.0$  and  $0.6$  at different temperatures in the critical-temperature region. It displays impressingly that different time scales govern the dynamic behavior in pure and disordered spin systems. It demonstrates clearly that only very long simulations yield reliable results. The relaxation time into thermal equilibrium starting from the purely magnetized state increases with dilution. Systems with concentrations  $p=1.0, 0.9$ , and  $0.8$  relax within the first 5000–10 000 lattice updates, depending on the distance to the critical temperature. Strongly diluted systems with  $p=0.6$  and  $0.5$  necessitate even larger times to equilibrate: 30 000–100 000 lattice updates.

In order to save computing time, measurements have

been performed only every 6–64 updates of the whole lattice. This avoids sampling highly correlated data. The time distance for measurements was estimated in preliminary runs following the heuristic procedure of Friedberg and Cameron:<sup>18</sup> Averages  $A_m$  are calculated taking only every  $m$ th measured value; the statistical error  $\Delta A_m$  determined for every  $m$  first increases with  $m$  until it reaches an approximately constant value at some  $m^*$ , which is a measure of the time distance between nearly uncorrelated measurements. As a result of these measurements, the time distance between successive measurements in our long runs has been chosen between 6 and 32 lattice updates for  $p=0.8$ – $1.0$  and between 16 and 64 lattice updates for  $p=0.5$  and  $0.6$ .

The number of Monte Carlo steps per spin (MCS) for each data point depends very much on the concentration and on the distance  $t$  from the critical temperature. Systems with concentrations  $p=1.0, 0.9$ , and  $0.8$  have been simulated with an accuracy between 50 000 and 300 000 MCS per data point, thus sampling about 10–20 000 nearly uncorrelated measurements. This is a factor 20 more than previous studies<sup>12–14</sup> in this concentration range. The concentrations  $p=0.6$  and  $0.5$  are even more demanding in simulation times. To obtain results of comparable accuracy as in the high-concentration range, simulation times between 300 000 and 1.2 million MCS were needed for each data point.

The error of each data point was determined by subdividing the whole Monte Carlo sequence into subsequences large enough to sensibly calculate subaverages. The error of the average over all subsequences was then estimated by the Gaussian error formula. Clearly, this way of error estimation works only when a large number of measurements are available. The errors enter the estimator of our fit so that less accurate data point have less weight in the fitting procedure. We point out that the errors determined in this way are over a magnitude larger than those determined in our analysis of correlations above. This indicates that one should be very careful when estimating errors of simulations; it is advisable to use different methods and regard the maximum error to be the true error.

The enormous simulation sequences of  $O(10^6)$  MCS demanded by disordered systems have prohibited simulations for a long time. However, the simulation times could be reduced by hardware developments and by an improvement of the multispin coding variant by Bhanot, Duke, and Salvador<sup>19</sup> that allows us to perform time-consuming simulations of discrete spin systems. Starting from a program of Ito and Kanada<sup>20</sup> for the pure Ising system, we have further improved the simulation speed arriving at a speed of 335 million spins per second on a single processor of the Cray YMP.<sup>21</sup> This is by now the fastest program comparing speeds on the same machine. The program simulates 64 systems with  $L^3$  sites and periodic-helical boundary conditions. The program is written in Fortran 77 and is fully vectorizable. In the simulation of diluted Ising systems the speed is reduced to 235 million spins per second since the update algorithm has to treat six nontrivial spin flip decisions compared to three in the pure case. Despite this high simulation

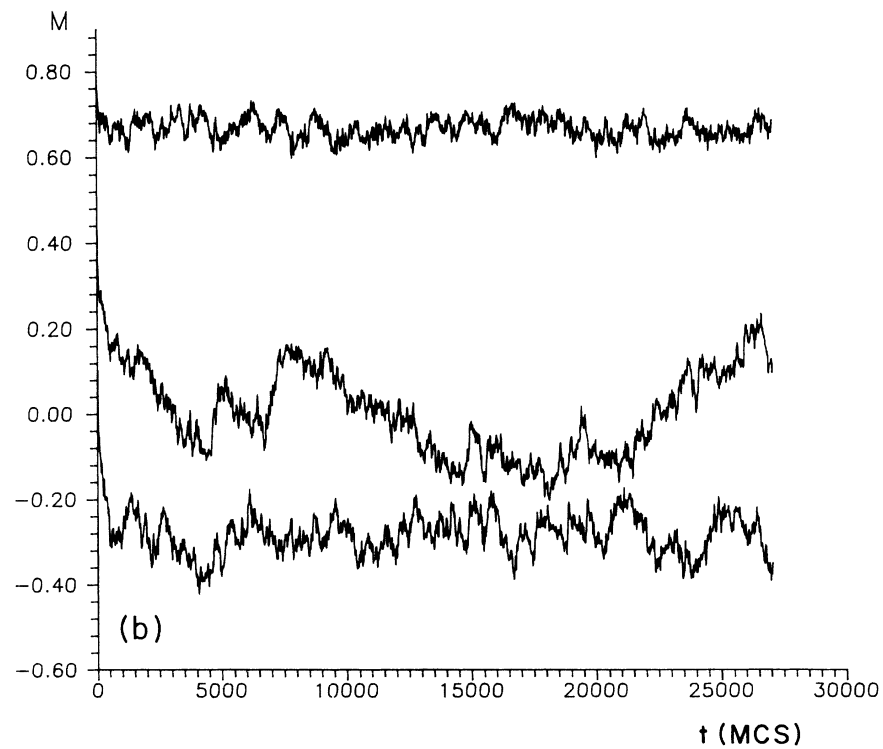
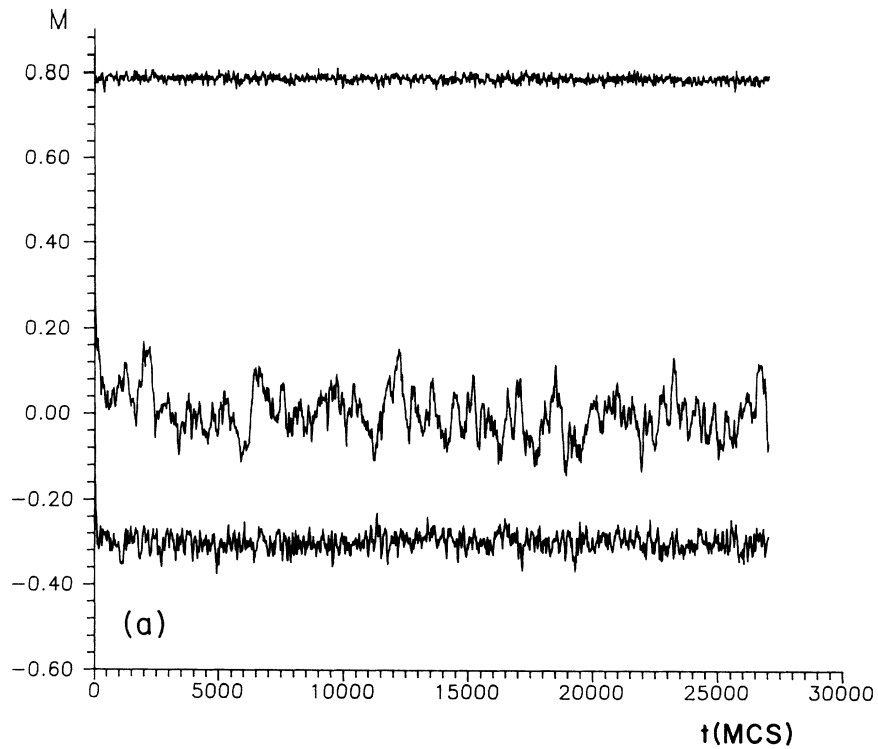


FIG. 2. Magnetization relaxation into thermodynamic equilibrium of  $60^3$  Ising systems with concentration  $p=1.0$  (a) and  $p=0.6$  (b). The time is measured in MCS (Monte Carlo steps per spin). The graphs in the middle correspond approximately to the critical temperature ( $T \approx T_c$ ). The upper and lower graphs in each figure correspond to reduced temperatures  $(T - T_c)/T_c \approx -0.02$  and  $0.02$ , respectively; these curves are displaced vertically by  $\Delta M = +0.3$  and  $-0.3$ , respectively, in order to fit all graphs into one figure. Comparison of the graphs shows the increased time scales in disordered spin systems.

speed our simulation needed about 200 h on the Cray XMP/YMP.

### III. RESULTS

We have tested our program by means of a simulation of the pure two-dimensional Ising system. In order to test not only the program but also our fitting procedure for the determination of critical exponents, we have chosen similar relative temperature distances  $t = (T - T_c) / T_c$  as in the diluted three-dimensional system. The temperatures were almost equally distributed on the  $\log_{10} t$  scale in the critical region. They were chosen in such a way that finite-size effects were negligible. Data points lying incidentally in the finite-size region ( $\xi \simeq L$ ) were discarded from the fitting procedure. The finite-size region can be easily identified by a curvature in the log-log plots (Fig. 3) towards the finite-size-dependent maxima  $\chi_0(L)$  as theoretically expected.<sup>16,17</sup> These finite-size effects were systematically studied also simulating smaller systems with  $L=30$  and  $40$ . In this finite-size region (below  $T_c$ ) the system frequently changes the sign of  $M$  (1). Clearly, these data have been discarded from the analysis. Figure 3 shows the log-log plots of the susceptibility obtained from a simulation of a  $250^2$  system (12 000 measurements taken every 250 updates of the lattice). The graphs show that finite-size effects are more pronounced in the ordered phase  $T < T_c$  than in the disor-

dered phase  $T > T_c$ . This effect can be observed in three dimensions and in disordered systems as well. Thus, one may approach the critical point more closely from the high-temperature phase  $T > T_c$ . From our test simulation of the two-dimensional Ising system we found  $\gamma = 1.76 \pm 0.01$  and  $\beta = 0.123 \pm 0.003$ , which is in good agreement with the exact values. The critical temperature  $T_c = 2.271 \pm 0.002$  of the  $250^2$  system is slightly larger than the exact value ( $T_c = 2.269$ ); this is a finite-size effect of the form  $T_c(L) = aL^{-\nu}$ .

Simulations with disordered Ising systems have been performed at the concentrations  $p = 1.0, 0.9, 0.8, 0.6,$  and  $0.5$ . In the critical region  $5 \times 10^{-3} < |t| < 10^{-1}$  we have chosen about 40 temperatures to have a dense sequence of data points. Figure 4 shows typical raw data of the susceptibility and specific heat of disordered systems with concentrations between  $p = 1.0$  and  $p = 0.5$ . Note that strongly disordered systems show a well-defined phase transition with a sharp singularity of the susceptibility. On the contrary, the specific heat becomes very narrow as the concentration decreases. The cusplike structure of the specific heat indicates a clearly negative value of the critical exponent  $\alpha$ .

The main problem in the determination of the critical exponents is undoubtedly a precise determination of the critical temperature. Once  $T_c$  is known, critical exponents can be determined in a straightforward way. We therefore first analyze the susceptibility that is the most

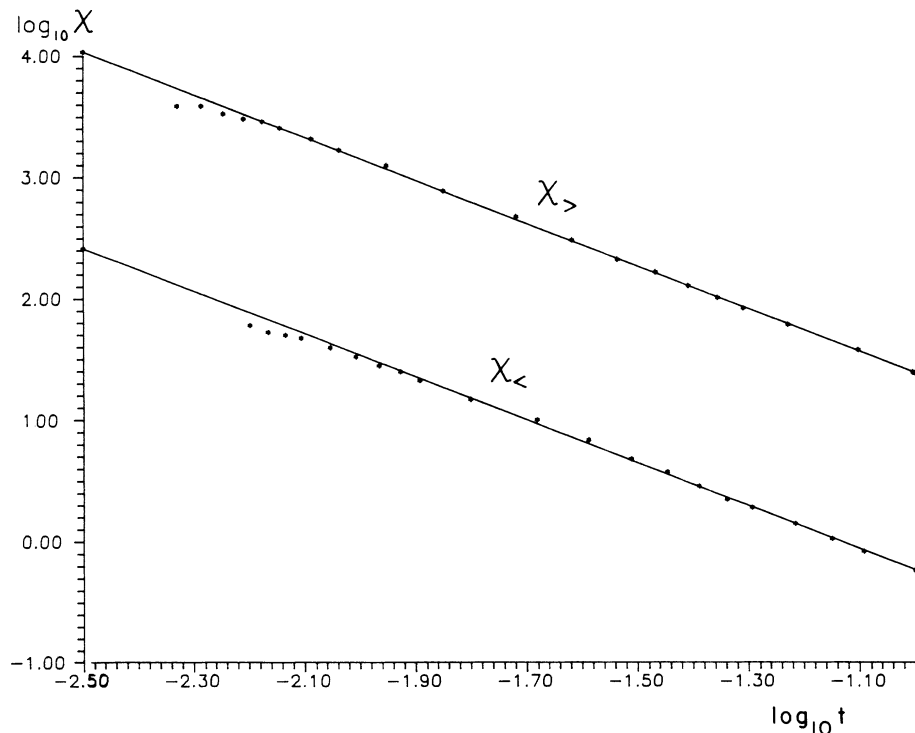


FIG. 3. log-log plot of the susceptibility of the two-dimensional Ising system. The fit of the data above and below  $T_c$  leads to  $T_c = 2.271$  and  $\gamma = 1.76 \pm 0.01$ . Note that a systematic decrease from the straight line occurs near  $T_c$ . The susceptibility approaches a size-dependent constant value  $\chi(L)$  at  $T_c$ . This crossover to finite-size behavior is more pronounced below  $T_c$  than above  $T_c$ .

sensitive quantity to the location of  $T_c$ . It is reasonable to fit the data simultaneously to the susceptibility  $\chi = C_+ t^{-\gamma}$  above and  $\chi = C_- (-t)^{-\gamma'}$  below  $T_c$  imposing the condition  $\gamma = \gamma'$ . This is a minimal constraint and has to be fulfilled if there is scaling at all. We have analyzed the data of each configuration separately in order to check for configuration-dependent effects. The critical temperature of each sample can be determined with a relative accuracy of  $2 \times 10^{-4} - 5 \times 10^{-4}$  for all concentrations. In addition to the standard thermodynamic quantities we have studied the fourth and sixth cumulant of the magnetization. These cumulants show a well-defined jump at  $T_c$ , which serves as an additional check for the correct value of  $T_c$ .<sup>15-17</sup> The critical exponents  $\gamma$  (Table I) determined from these fits have an error of approximately 0.01 for  $p \geq 0.8$ . The log-log plots (Fig. 5) of our  $\chi$ ,  $m$ , and  $\Gamma$  data show that the expected power-law behavior holds with constant exponents over the temperature interval  $(t_l, t_u)$  (Table I). As shown in Fig. 6 the exponent  $\gamma$  increases with disorder even in the range of weak dilution. The exponents nearly lie on a straight line, leading from  $\gamma = 1.24 \pm 0.01$  ( $p = 1.0$ ) over  $1.30 \pm 0.01$

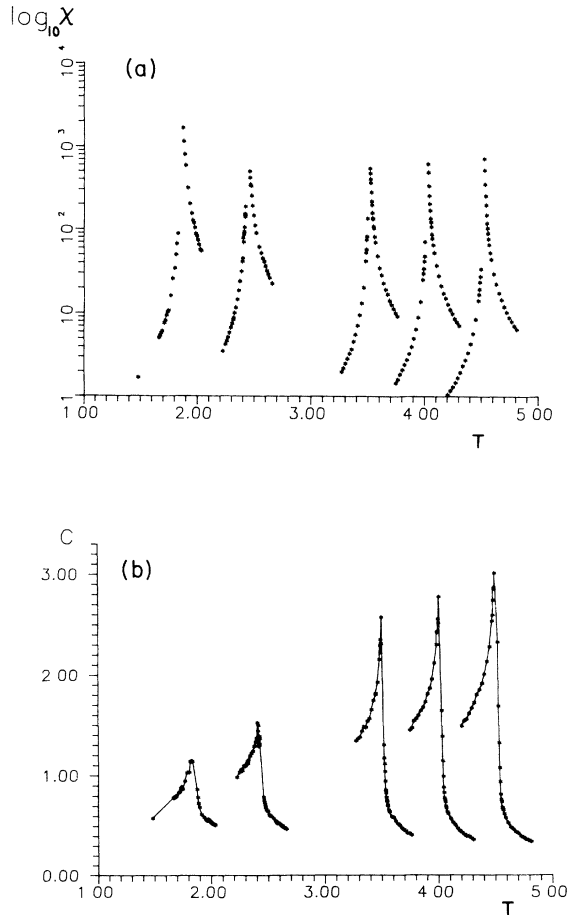


FIG. 4. Typical raw data of the susceptibility (a) and the specific heat (b) of disordered systems. The concentrations are from left to right:  $p = 0.5, 0.6, 0.8, 0.9$ , and  $1.0$ . Note that the strongly diluted systems have a pronounced singularity in the susceptibility, but a narrow and cusplike specific heat.

TABLE I. Critical exponents  $\gamma$ ,  $\beta$ , and  $\zeta$  and universal amplitudes for systems with different concentrations.  $C_+$ ,  $C_-$  and  $A$  are the amplitudes of the susceptibility and the magnetization.  $t_l$  and  $t_u$  are temperatures explained in the text.

$p$	$T_c(p)/T_c(1)$	$\gamma$	$C_+/C_-$	$\beta$	$A$	$\zeta$	$\zeta = 1 - \beta$	$\alpha = 2 - 2\beta - \gamma$	$t_u$	$t_l$
1.0	1.0000	$1.24 \pm 0.01$	$5.5 \pm 0.05$	$0.305 \pm 0.01$	$1.51 \pm 0.03$	$0.690 \pm 0.01$	$0.695 \pm 0.01$	$0.15 \pm 0.03$	$4 \times 10^{-2}$	$5 \times 10^{-3}$
0.9	0.8889	$1.30 \pm 0.01$	$5.4 \pm 0.1$	$0.315 \pm 0.01$	$1.49 \pm 0.02$	$0.690 \pm 0.02$	$0.685 \pm 0.01$	$0.07 \pm 0.03$	$5 \times 10^{-2}$	$5 \times 10^{-3}$
0.8	0.7760	$1.35 \pm 0.01$	$5.1 \pm 0.1$	$0.330 \pm 0.01$	$1.49 \pm 0.01$	$0.680 \pm 0.01$	$0.670 \pm 0.01$	$-0.01 \pm 0.03$	$5 \times 10^{-2}$	$9 \times 10^{-3}$
0.6	0.5377	$1.48 \pm 0.02$	$5.5 \pm 0.1$	$0.330 \pm 0.01$	$1.37 \pm 0.02$	$0.690 \pm 0.01$	$0.670 \pm 0.01$	$-0.14 \pm 0.04$	$10^{-1}$	$2 \times 10^{-2}$
0.5	0.4098	$1.49 \pm 0.02$	$5.6 \pm 0.1$	$0.335 \pm 0.01$	$1.31 \pm 0.02$	$0.675 \pm 0.01$	$0.665 \pm 0.01$	$-0.16 \pm 0.04$	$10^{-1}$	$2 \times 10^{-2}$

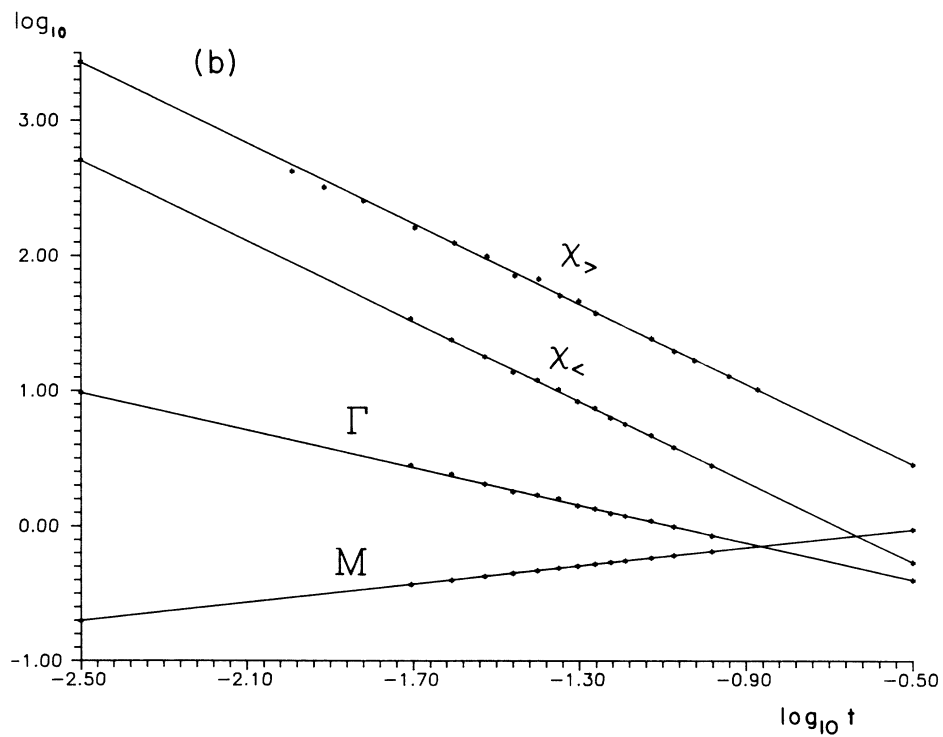
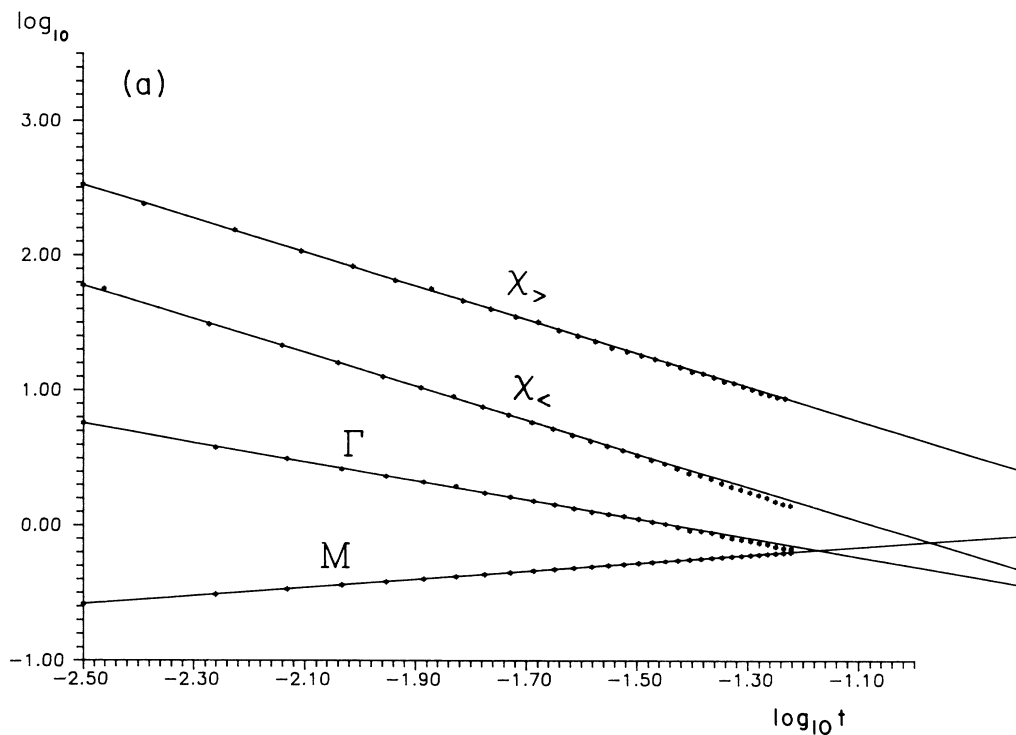


FIG. 5. log-log plots of the susceptibility  $\chi$  above and below  $T_c$ , magnetization  $M$  and magnetization-energy correlation function  $\Gamma$  below  $T_c$  of the pure system  $p=1.0$  (a) with  $\gamma=1.24$ ,  $\beta=0.305$ , and  $\zeta=0.69$  and of a diluted system ( $p=0.6$ ) (b) with  $\gamma=1.48$ ,  $\beta=0.33$ , and  $\zeta=0.68$ . The plots show that corrections to scaling lead to curvatures in the noncritical region, which affect the quantities in a different way.

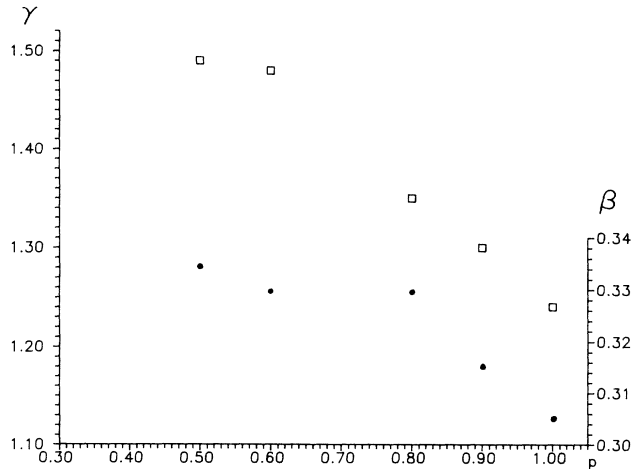


FIG. 6. Effective critical exponents  $\beta$  (dots) and  $\gamma$  (squares) for disordered Ising systems with different concentrations  $p$ . Both exponents show a strong increase in the weak-disorder regime and reach asymptotic values  $\beta=0.335$  and  $\gamma=1.49$  at  $p=0.5$ .

( $p=0.9$ ) to  $1.35\pm 0.01$  (Fig. 6). In the strongly disordered concentration range  $p < 0.8$ , the increase of  $\gamma$  proceeds with the same slope up to  $\gamma=1.48\pm 0.02$  ( $p=0.6$ ) and reaches a plateau value  $\gamma=1.49\pm 0.02$  at  $p=0.5$ . The error of  $\gamma$  for  $p=0.6$  and  $p=0.5$  is about 0.01–0.03 for each configuration. In this strongly disordered case, the configuration-dependent variations of  $\gamma$  are clearly larger than the error of each configuration. For  $p=0.6$ , we find  $\gamma$  values between 1.45 and 1.52 and for  $p=0.5$  the values of  $\gamma$  are between 1.46 and 1.53. These differences are not surprising; even a  $60^3$  system is far away from the thermodynamic limit. Averaging over all configurations leads to an approximate error of 0.01–0.02 (Table I). The universal amplitude ratio  $C_+/C_-$  of the pure system is  $5.5\pm 0.05$ . The ratio first decreases upon dilution and reaches a minimum value of  $5.1\pm 0.1$  at  $p=0.8$ . Upon further dilution into the strongly disordered regime  $C_+/C_-$  increases again and reaches  $5.6\pm 0.1$  at  $p=0.5$ , a value very near to the pure case.

The magnetization data are fitted to the power law  $m = A(-t)^\beta$  with  $T_c$  fixed from the susceptibility measurements. The critical exponent  $\beta$  is comparatively stable against variations of  $T_c$  within reasonable bounds. The values of  $\beta$  thus obtained (Table I) have an error of about 0.01. Our pure system value is  $\beta=0.305$ , which is lower than the theoretically expected value 0.32. This systematic shift to lower values has also been observed in previous simulations.<sup>13,14</sup> We suspect that the periodic boundary conditions that allow for domains extending beyond the systems boundary are responsible for this effect. Indeed, we have performed simulations with self-consistent boundary conditions (same system size, same temperatures, same random number sequence) and have obtained the correct value  $\beta=0.32\pm 0.01$ . However, self-consistent boundary conditions have disadvantages,

which will be discussed in a separate paper. The concentration dependence of  $\beta$  is quantitatively not as remarkable as the concentration dependence of  $\gamma$ . However, the increase of  $\beta$  is very similar to  $\gamma$ ;  $\beta$  also reaches a plateau value  $\beta=0.335$  at  $p=0.5$ . The universal amplitude  $A$  of the magnetization shows a monotonical decrease from  $A=1.51\pm 0.03$  ( $p=1$ ) to  $A=1.31\pm 0.02$ .

The determination of the exponent  $\zeta$  is unfortunately not as precise as the determination of  $\beta$ , since  $\Gamma$  shows more curvature in the  $\log_{10}\Gamma$ - $\log_{10}t$  plots than the magnetization [Fig. 5(a)]. Scaling corrections are responsible for this curvature in the crossover region to noncritical behavior. We point out that there are configurations that show pronounced curvature in this temperature region; other configurations hardly show any deviation from the power law [Fig. 5(b)]. The accuracy of  $\zeta$  (Table I) is between 0.01 and 0.03. We find that  $\zeta=0.69\pm 0.01$  for the pure Ising systems. In the strongly disordered regime,  $\zeta$  decreases to 0.675 at  $p=0.5$ . The comparison of the values of  $\beta$  with those of  $\zeta$  (Table I) shows that the scaling relation  $\zeta=1-\beta$  (12) is fulfilled within the error bounds. Thus, the scaling relation (12) is very useful in proving scaling behavior.

The quantitative analysis of the specific-heat data is problematic as Fig. 4 shows. Even in the case of *weak* dilution the singularity is very weak and next-to-leading and regular terms are important. We have therefore calculated the values of  $\alpha$  in Table I by means of the Rushbrooke equation;  $\alpha$  approaches a limiting value of  $-0.16\pm 0.04$ . The specific-heat data at  $p=0.6$  and 0.5 show their maximum value slightly displaced from  $T_c$ . For  $p=0.6$  this maximum is at  $t=-0.015\pm 0.005$ , and for  $p=0.5$  it is at  $t=-0.022\pm 0.008$ . This displacement of the specific-heat maximum has been observed in many experiments in the past; it is not an effect of the Monte Carlo simulation.

Summarizing, we have found that the critical behavior of spin systems is clearly affected by disorder in all measured quantities. The most important effect of disorder occurs in the susceptibility. The exponent  $\gamma$  depends on the concentration and increases from its pure system value  $\gamma=1.24\pm 0.01$  to  $\gamma=1.49\pm 0.02$ . The critical exponents  $\beta$  and  $\zeta$  show a similar dependence and reach  $\beta=0.335\pm 0.01$  and  $\zeta=0.675\pm 0.01$  in the strong-disorder regime. The critical exponents do not show a variation with temperature. However, the interval is about one decade on the  $\log_{10}t$  scale. This may be too small to detect variations in  $\gamma$  significantly larger than the errors. Our results are in good agreement with recent Monte Carlo simulations of the diluted Ising model by Wang and Chowdhury<sup>22</sup> who simulated even larger systems with the Swendsen-Wang dynamics. These authors measured the susceptibility above  $T_c$  and found  $\gamma=1.52\pm 0.07$  for strongly diluted systems. Wang and Chowdhury originally found a temperature dependence of their results for  $\gamma$ . In an extensive simulation for  $p=0.8$  this effect was shown to be a crossover to noncritical behavior.<sup>23</sup> Their new result  $\gamma=1.36$  for  $p=0.8$  is in excellent agreement with our own value  $\gamma=1.35$  for this concentration.

The interpretation of Monte Carlo and other experimental data concerning critical behavior is a difficult



matter since data can be sampled only in a very limited temperature range ( $t_l, t_u$ ) above as well as below  $T_c$  [ $t = (T - T_c)/T_c$ ].  $t_l$  is at most of the order  $10^{-3}$  since increasing simulation times and finite-size effects prevent approaching the critical point further. The upper bound  $t_u$  is the relative temperature above which nonuniversal behavior becomes important. Nonuniversal behavior has been observed as a curvature in the log-log plots for larger distances to  $T_c$  in the magnetization, susceptibility, and the magnetization-energy correlation data (Fig. 5).

We have found that the exponents in the critical-temperature range are concentration but not temperature dependent. This does *not* mean, however, that there are many different critical points or even a line of critical points each describing the asymptotic behavior of a spin system with some concentration. The exponents of diluted systems determined in the temperature range ( $t_l, t_u$ ) (Table I) are not asymptotic exponents but effective critical exponents. Effective exponents characterize the critical behavior in the observed temperature range.<sup>24</sup> We expect that the effective exponents we have measured may be calculated within an advanced theory that is able to describe critical phenomena for systems with any degree of disorder. The existing theories for systems with *weak* disorder and for percolation-dominated critical behavior should appear as limiting cases of such a theory.

Concerning the *weak* disorder regime we conclude that the critical behavior is changed in all quantities when dilution sets in (Fig. 6). Moreover, the quantitative changes are very pronounced and beyond any doubts. This result contradicts the theoretical belief based on the small crossover exponent  $\phi_x$  that impure critical behavior is unobservable in experimental temperature ranges. However, one cannot expect the renormalization group to give quantitatively correct answers concerning nonuniversal properties. Nevertheless, the strong increase of  $\gamma$  up to values around 1.50 is not explained by the conventional

theory of weak disorder, which predicts a change to  $\gamma = 1.335$ .<sup>5</sup> There may be at least two reasons for this failure. The first possibility is that the conventional theory<sup>1-5</sup> describes only the asymptotic properties in a correct way—thus it would not be possible to prove its correctness experimentally or by simulation. The second possibility is that the theory is valid only for nearly pure systems. We shall test the second possibility by means of further simulations of very weakly disordered systems between  $p = 0.9$  and  $p = 1.0$ .

In the strongly diluted range we find a parallel concentration-dependent increase of  $\beta$  and  $\gamma$  to plateau values 0.335 and 1.49 at  $p = 0.5$ . This is half-way to the critical exponents  $\gamma = 1.7$  (dilute  $s$ -state Potts-model) and  $\gamma = 1.5$  (dilute  $n$ -vector models) expected at the percolation threshold.<sup>9</sup> A quantitatively reliable description from the simplified approaches at  $p_c$  (Refs. 7-10) cannot be expected in the medium-concentration range around  $p = 0.6$  where our simulations were performed. Unfortunately, further simulations near the percolation concentration  $p_c = 0.31$  become increasingly time consuming since one has to simulate larger and larger systems to avoid configuration dependencies. It is therefore at present not possible to approach the percolation concentration more closely in order to further investigate the crossover to percolation-dominated exponents. We expect that a theory which incorporates both the *weak*- and *strong*-disorder limit will satisfactorily explain the findings of the present Monte Carlo study.

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