Crossover phenomena in disordered two-dimensional Ising systems: A Monte Carlo study

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We performed extensive Monte Carlo simulations of site-disordered two-dimensional Ising systems along the critical line $T_c(p)$ in the concentration range of magnetic sites between $p=0.6$ and $p=1.0$ ($p_c=0.59$). Magnetic and caloric properties were studied as well as the cumulants of the magnetization distribution. We found that the disorder induces a crossover phenomenon in the experimental temperature range which leads to a strong, concentration-dependent increase of γ_{eff} ($\gamma_{\max}=2.16$ for $p=0.7$) in the temperature range $10^{-2}<(T-T_c)/T_c<10^{0}$. Near T_c, γ_{eff} asymptotically approaches $\gamma=1.75$, independent of the concentration. We propose a model of weakly coupled compact clusters of spins to describe this crossover phenomenon.

There is a long-standing research interest in critical phenomena in disordered spin systems. The main question is how the disorder changes the nature of the phase transition and thereby the universality class.[1] The asymptotic critical behavior may be changed in three different ways: (i) The disorder may be an irrelevant perturbation so that the critical behavior is asymptotically unchanged; (ii) the disorder may be relevant and lead to a different universality class; and (ii) in rare cases, the disorder may lead to critical exponents which depend continuously on the concentration. Heisenberg systems belong to the first category; their crossover exponent ϕ_x with respect to disorder is equal to the critical exponent of the specific heat of the pure system $\alpha_h=-0.09$; thus the disorder is asymptotically irrelevant.[2-4] In three-dimensional Ising systems, the disorder is a relevant perturbation leading to a different universality class: The set critical exponents change from ($\alpha=0.11$, $\beta=0.325$, $\gamma=1.24$ $\nu=0.63$) to ($\alpha=-0.01$, $\beta=0.34$, $\gamma=1.32$, $\nu=0.67$).[5-7] These results confirm the heuristic Harris criterion:[1] Disorder is relevant, if $\nu_h<2/d$, which is equivalent to $\alpha_h>0$ if hyperscaling is valid. The two-dimensional Ising system is marginal in this respect since its correlation length diverges with $\nu_h=1$ and the specific heat with $\alpha_h=0$, respectively. Recent work based on conformal invariance[7-12] methods have led to predictions for the bond-diluted two-dimensional Ising system: The critical exponents ($\alpha=0$, $\beta=\frac{1}{8}$, $\gamma=\frac{7}{4}$, $\nu=1$) remain unchanged—disorder leads to logarithmic corrections only; e.g., the susceptibility diverges as $\chi\sim t^{-7/4}|\ln t|^{7/4}$, the magnetization becomes $M\sim t^{1/8}|\ln t|^{-1/16}$, and the specific heat gets a double-logarithmic form.[7-11]

It must be stated clearly that the validity of all results[1-12] is restricted in two ways: (i) All approaches are restricted to weak disorder since disorder is treated as a perturbation of the pure system—it is not clear what weak disorder means; (ii) all results are valid asymptotically near the critical point—there is no measure where this asymptotic regime is reached on experimentally accessible concentration and temperature scales.

Complementary approaches to critical phenomena in disordered spin systems have started from the opposite limit, i.e., from the percolation fixed point,[13-15] where long-range order breaks down. Exploiting the scale invariance at p_c, the critical behavior has been studied on fractal models having similar fractal dimensions as the percolating cluster.[16,17] In the framework of the links-nodes-blobs model, it has been shown that percolation exponents (e.g., $\alpha=-\frac{2}{3}$, $\beta=\frac{5}{36}$, $\gamma=\frac{43}{18}$, $\nu=\frac{4}{3}$ in $d=2$) determine the critical behavior of the spin system at p_c with a crossover exponent $\phi_t=1$ with respect to thermal fluctuations valid in all dimensions for discrete spin models.[18] However, the assumption of one-dimensional thermal correlations restricts this result to the vicinity of the percolation point.

Summarizing, the theoretical predictions are valid only asymptotically near T_c and in two opposite extreme cases—a theoretical link between them does not exist. On general grounds one expects a crossover between the fixed point calculated for weak disorder and the percolation fixed point. This crossover must show up in concentration- and temperature-dependent effective exponents. In addition, experiments and simulations may not be performed in the asymptotic regime, so that an additional crossover due to scaling corrections or unstable (non asymptotic) fixed points may arise. These aspects are relevant if one tries a comparison of experiments and simulations with the asymptotic theories.

The increasing computational power and refined algorithms have led to a number of simulations of disordered spin systems.[19-22] In three dimensions simulations have been performed systematically down to $p=0.5$ ($p_c=0.31$). It has been shown that the critical behavior changes continuously with concentration: $\bar{\gamma}$ increases up to $\bar{\gamma}=1.49\pm0.02$, whereas $\bar{\beta}$ increases up to $\bar{\beta}=0.34\pm0.01$.[21,22] These exponents describe the susceptibility and magnetization in the temperature range $5\times10^{-3}\le t\le10^{-1}$ by a fit to the usual power law. Effective exponents, obtained for $p=0.8$,[20] show a temperature dependence. Thus simulations are not in the asymptotic temperature range—a quantitative comparison with asymptotic theoretical results is hardly possible. In two dimensions finite-size simulations of the weakly bond-diluted Ising system[23,24] have been performed re-

TABLE I. Critical-size study ($\xi \gg L$); $\bar{\gamma}$ is the averaged exponent determined in the critical region $10^{-2} \leq t \leq 10^{0}$ ($\xi \ll L$).

p	$T_c(p)/T_c(1)$	U^*	γ/ν	$\bar{\gamma}$	β/ν
1.00	1.0000	0.613(3)	1.75(1)	1.74	0.125(5)
0.95	0.9203	0.626(3)	1.75(2)	1.79	0.125(5)
0.90	0.8375	0.630(5)	1.76(2)	1.88	0.125(5)
0.85	0.7523	0.628(4)	1.76(2)	1.96	0.12(1)
0.80	0.6645	0.620(8)	1.78(2)	2.07	0.11(1)
0.75	0.5694	0.625(10)	1.80(3)	2.11	0.10(2)
0.70	0.4738			2.16	

cently, confirming that $\gamma/\nu = \frac{7}{4}$ and $\beta/\nu = \frac{1}{8}$.[7,9–11] A verification of the double-logarithmic specific heat has also been stated.[23,24] However, the crossover from a lnL to a ln lnL behavior is difficult to detect in view of finite-size corrections which should be included for the small lattice sizes.

In the present Monte Carlo study, we investigate a two-dimensional Ising model with site disorder on a square lattice ($p_c = 0.59$) of size L ($72 \leq L \leq 250$) with concentrations p between $p = 0.6$ and 1.0. We used the canonical Monte Carlo method, i.e., single spin-flip dynamics in a heat bath with fixed temperature, to obtain data from the Gibbs ensemble. We implemented a fast code on the Cray Research, Inc, Y-MP vector computer which runs at 450×10^6 spin updates per second on a single CPU.[26] In preliminary runs we tested the initial relaxation of two-dimensional diluted systems and estimated the approximate location of the critical points $T_c(p)$. Simulations of lattices with size 72^2, 100^2, 124^2, and 250^2 were then performed for a finite-size analysis.[27] The typical run length was $(2-5) \times 10^6$ lattice updates for the 250^2 lattice. The first 50 000 to 300 000 lattice updates were discarded to reach thermodynamic equilibrium. In order to avoid sampling highly correlated data, we made measurements only every 50–200 updates of the lattices. We sampled data of the magnetization, susceptibility, and specific heat defined in the usual way via fluctuations[22] of energy and magnetization. For the fixed-point analysis and the determination of T_c, we calculated the cumulants

$$U_L = 1 - \langle M^4 \rangle / 3 \langle M^2 \rangle^2$$

and

$$V_L = 1 - \langle M^4 \rangle / 2 \langle M^2 \rangle^2 + \langle M^6 \rangle / 30 \langle M^2 \rangle^3 ,$$

of the magnetization. Our finite-size simulations were performed at about 15 temperatures in the immediate vicinity of the critical point ($\xi \gg L$); the critical temperature T_c was finally determined by the intersection of the cumulants for different lattice sizes.[27] The corresponding sixth-order cumulants did not give additional information on T_c. For each concentration we collected data from 30–40 configurations, even for $L = 250$. Similarly, we studied the other system sizes $L = 100$ and 124 to derive T_c from the intersection with a relative statistical error of 0.0005–0.001. We found that even for these large lattices there is still a small finite-size shift of 10^{-3} in the values of T_c. The magnetization and susceptibility have been averaged over independent configurations; the errors of these quantities have also been derived from this configurational average. The data have a relative error of $5 \times 10^{-3} - 2 \times 10^{-2}$, which is larger than the statistical error of the data for each configuration determined from the variance of subaverages. The values of γ/ν and β/ν (Table I) were obtained via the usual finite-size scaling[27] of the magnetization and susceptibility. We have found agreement calculating exponents with different lattice

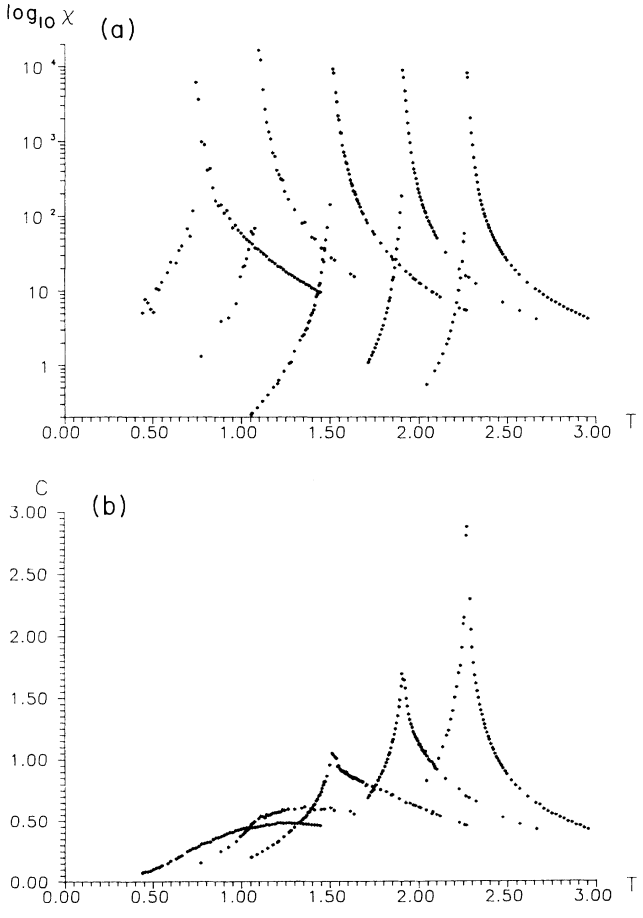

FIG. 1. Raw data of the susceptibility χ on a semilogarithmic plot and of the specific heat C in a linear plot for samples $p = 0.6$, 0.8, and 1.0 as a function of temperature. Note that the specific-heat singularity is more and more suppressed with increasing dilution, whereas the susceptibility diverges strongly. For $p \leq 0.7$ the singularity of c is vanishingly small; only a regular contribution remains.

sizes within the statistical errors of our exponent estimates. Both exponents show a slight but systematic dependence on the concentration which is almost within the error bounds. This is a residual effect of the crossover as will be explained below. It should be mentioned that U^* increases abruptly from the pure system value $U^*(p=1)=0.613\pm0.003$ to $U^*(p\neq1)=0.625\pm0.005$. However, this splitting is not large enough compared with our errors for U^* to draw a conclusion about a splitting of the fixed points.

Our second set of simulations was performed with the $L=250$ lattice in the usual critical temperature region $10^{-2}<|t|<10^{0}$ ($\xi<L$) excluding the finite-size region (Fig. 2) ($t=(T-T_c)/T_c$). We typically simulated 6 configurations at each concentration with a dense sequence of about 60 temperatures above and below T_c collecting all relevant magnetic and caloric data. The length of each simulation was $(2-6)\times10^6$ updates after reaching equilibrium. As can be seen from our raw data (Fig. 1), strong critical magnetization fluctuations are accompanied by weak energy fluctuations when disorder is increased. Note that below $p=0.7$ the singularity of the specific heat even vanishes, whereas the susceptibility diverges as strong as in the pure system. We restricted the main part of the analysis to the concentrations $p=0.7-1.0$ since the lower concentrations $p=0.6$ and 0.65 need such a large amount of computing time that we were not able to produce statistically acceptable data for the determination of critical exponents. Some typical data of the susceptibility above T_c after averaging over configurations are shown in Fig. 2. The magnetization and susceptibility were fitted to their power-law behavior $M=A|t|^{\bar\beta}$ and $\chi=Ct^{-\bar\gamma}$ using the critical temperatures $T_c(p)$ determined previously (Table I). As Fig. 2 shows, one has to avoid carefully the crossover to finite-size-affected data. The critical exponents $\bar\gamma$ and $\bar\beta$ determined in that way grossly characterize the critical behavior in the temperature range $10^{-2}\leq t\leq10^{0}$. $\bar\beta$ does not change notably with dilution within the errors and is in accord with the values of our finite-size analysis assuming $\nu=1$[7–11] However, $\bar\gamma$ increases drastically with dilution up to $\bar\gamma=2.16$ at $p=0.7$ (Table I, Fig. 2). We conclude that the critical behavior in the region $\xi\ll L$ is different from the critical behavior at T_c where $\xi\gg L$. We analyzed this crossover from the outer (transient) critical region to the inner (asymptotic) critical region by calculating the effective exponent $\gamma_{\rm eff}(t)$ (Ref. 25) as the local logarithmic derivative of the susceptibility by means of a least-squares fit of our data in small temperature intervals. The results are shown in Fig. 3. In the pure system there is a slight increase of $\gamma_{\rm eff}(t)$ until the critical exponent reaches its asymptotic behavior $\gamma_{\rm eff}=1.75$, consistent with the value obtained by the finite-size analysis (Table I).[23] In diluted systems $\gamma_{\rm eff}$ behaves in a different way. The samples with $p=0.95$ and 0.90 show that $\gamma_{\rm eff}$ increases up to a concentration-dependent maximum value when approaching T_c and finally $\gamma_{\rm eff}$ decreases to reach the values determined by the finite-size scaling analysis. The temperature $t_{\rm max}$ where $\gamma_{\rm eff}$ reaches its maximum value increases with dilution. In fact, below

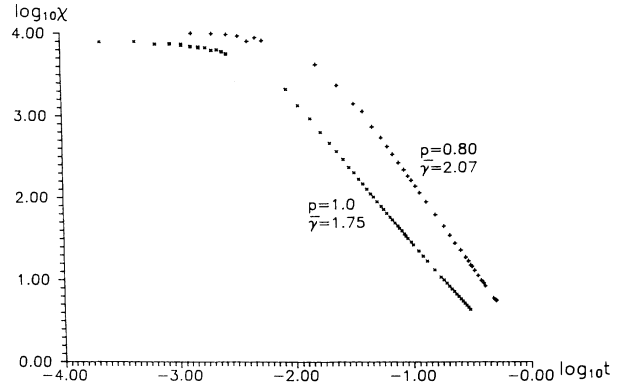

FIG. 2. Log-log plot of the susceptibility of a pure and of a diluted ($p=0.80$) system above $T_c(p)$. At a reduced temperature $t=10^{-2}$, the data begin to approach a finite-size-dependent maximum value $\chi_{\rm max}$ ($L=250$).

$p=0.90$ the increasing part of $\gamma_{\rm eff}(t)$ is outside the temperature range of our simulation. The width of the asymptotic regime depends on concentration in the way that more strongly diluted systems approach the asymptotic regime more closely to T_c; this explains the fact that the values of γ/ν (Table I) obtained from our finite-size analysis have a slight but systematic dependence on the concentration.

Summarizing, our simulations show a pronounced crossover, with a concentration- and temperature-dependent effective exponent $\gamma_{\rm eff}$ in a transient regime $10^{-2}\leq t\leq10^{0}$, which is the temperature range usually accessible for experimental investigations.[28] This crossover masquerades as a concentration- and temperature-dependent exponent. Asymptotically, we find the exponents of the pure and weakly disordered two-dimensional spin system. The validity of our results ex-

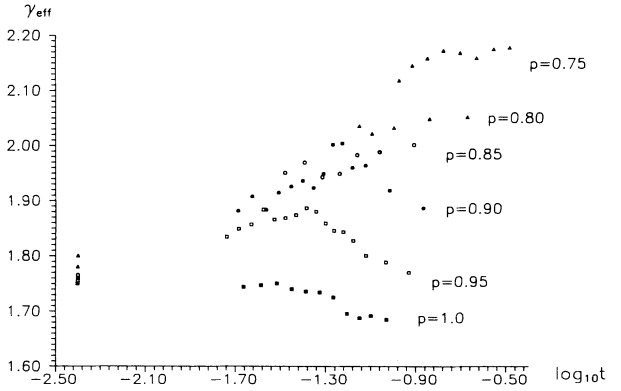

FIG. 3. Effective critical exponent $\gamma_{\rm eff}(t)$ as a function of the reduced temperature $t=(T-T_c)/T_c$ on a logarithmic scale. The data points displayed at about $\log_{10}(t)\sim-2.5$ are those of our finite-size study at $T_c(p)$ assuming the correctness of $\nu=1$ (Refs. 7–11).

tends down to considerable site disorder at $p=0.75$. The physical origin of the crossover phenomenon found in this work and presumably in three dimensions[19–22] may be explained heuristically by the following argument. The study of configurations of disordered systems[29] supports the idea that disordered systems are composed of compact clusters of spins of irregular shape with average size l_c. Inside these clusters the spins have almost the full connectivity of the pure system, apart from small isolated sites or group of sites which are not occupied. The clusters are loosely coupled to each other by few bonds so that a flip of an almost ordered cluster gives a large contribution to the susceptibility but a minor contribution to the specific heat (Fig. 1). On approaching the critical point $T_c(p)$ from above, critical spin ordering first proceeds within the clusters ($\xi \ll l_c$) for $T < T_c(p=1)$ (Griffiths phase); when the critical temperature $T_c(p)$ of the system is approached more closely, the clusters are nearly ordered ($\xi \simeq l_c$) and act as superspins coupled to each other by few surface spins of the clusters. The critically fluctuating clusters lead to a large susceptibility depending on the average volume v_c, but to a small specific heat depending on the surface s_c of the clusters. In the asymptotic regime ($\xi \gg l_c$), the concept of translationally invariant system applies again and the results of weak disorder are found. The links-nodes-blobs model,[18] which describes critical phenomena at the percolation point, is a natural limiting case of one-dimensionally coupled clusters in our model.

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