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LETTER TO THE EDITOR

Critical crossover phenomena in disordered Ising systems

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Abstract. We have investigated the critical behaviour of site-disordered Ising systems over a large range of dilution ($0.6 \leqslant p \leqslant 1.0$) investing about 10^{15} single spin flips with conventional local dynamics. Critical temperatures have been determined with high precision using the cumulant method. The finite-size simulations lead to concentration-dependent exponents which seem to violate universality. We show that the concentration dependence is induced by a crossover phenomenon which governs a large interval of the critical region. We find that the scaling functions of systems with different disorder converge asymptotically to universal behaviour consistent with the fixed point of weak disorder.

The influence of disorder on critical behaviour has been in dispute for a long time. Early renormalization group (RG) calculations based on weak randomness [1–3] have shown that a change of the universality class depends on the order parameter dimension n of the system. These results have confirmed the heuristic Harris criterion [4]. In more general works, it has been shown [5] that the naive form of this stability criterion ('stability depends on the exponent α of the pure system') applies only to simple energy-like coupling of disorder [1–3]. Other sorts of disorder like anisotropic coupling [5, 6], random-field coupling [7], extended [8, 9] and correlated defects [10] have been investigated.

In this letter we report simulations of the Ising model with classical site-disorder [1–3]. In the field-theoretic formulation site-disorder introduces a new spin-operator into the problem. A new stable fixed point with new exponents has been calculated for Ising systems ($n = 1$), whereas Heisenberg systems ($n = 3$) are uneffected by this kind of disorder. The identity of the crossover exponent ϕ with the exponent α of the pure system has been shown to all orders in perturbation series [11, 12]. Due to the $O(\epsilon^{1/2})$ random fixed point, critical exponents for the random Ising model are hard to calculate in comparison with the pure case [13]. The two-loop-order field-theoretic renormalization [14] has been extended recently up to four-loop order [15], leading to reliable results in three dimensions: $\beta = 0.348$, $\gamma = 1.321$, $\nu = 0.671$ and $\eta = 0.032$ for the random Ising model.

Since the crossover exponent ($\phi = \alpha = 0.11$) [16] is very small, it is expected that random exponents should be seen only very near the critical point in a region $t \ll t_x$. The crossover temperature $t_x \sim (1-p)^{1/\phi}$ on the reduced temperature scale $t = (T/T_c(p) - 1)$ depends on the concentration p of spins. A finite-size analysis

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is consequently expected to show random Ising exponents only for large systems $L \gg L_x$ with $L_x \sim (1-p)^{-\nu/\phi}$. Smaller lattices ($L \ll L_x$) should be dominated by the pure Ising exponents. We point out that a calculation of the crossover between the two fixed points has not been carried out so far.

The basic feature of the theoretical approaches to disorder [1–3, 11, 13, 15] is the assumption of weak disorder. This allows for a translational-invariant effective Hamiltonian of the disordered system. In this letter we address the open problem of what this restriction means for real systems. A closely related question [13] is the relevance of the percolation fixed point [17, 18] in the renormalization scenario of disordered systems. Although the percolation fixed point is unstable [19], it may be relevant for strongly diluted systems in the non-asymptotic regime. It has been stated earlier [13] that a complete theory for disorder phenomena in critical systems must include all three fixed points.

The simulation of disordered spin systems has long been hampered by strongly increasing relaxation times and the need to perform configurational averages [20]. Now, precise Monte Carlo results are possible by new cluster algorithms [21, 22] and refined vectorized implementations of local algorithms [23]. We have invested about 10^{15} single spin flips for the finite-size simulation of disordered Ising systems in the concentration range $p \geqslant 0.6$. This is more than has ever been done before in a classical statistical problem. Our fast vectorized Metropolis dynamics was used which yields a speed of 335×10^6 Monte Carlo steps (MCS) per second for the pure Ising model and 215×10^6 MCS/second for the site-diluted model [23]. Despite this speed, the project needed about 2000 CPU-hours on the CRAY Y-MP.

As a preliminary step, we have invested a large amount of computing time (4×10^{14} MCS/spin) for the determination of the critical temperatures $T_c(p)$. The cumulant method [24] has been applied to calculate $T_c(p)$ by the intersection of the fourth-order cumulants

$$U = 1 - \frac{\langle \mathcal{M}^4 \rangle}{3 \langle \mathcal{M}^2 \rangle^2} \tag{1}$$

of the magnetization density $\mathcal{M}$. To obtain highly resolved data, simulations were done in small temperature intervals ($|t| < 10^{-3}$) around the critical temperature $T_c(p)$ at 8–16 equidistant temperatures. In each run, we sampled $1\text{–}2 \times 10^6$ MCS/spin after an equilibration of 20 000–40 000 MCS/spin, which corresponds to more than $20\ \tau_{\mathrm{int},|M|}$, where $\tau_{\mathrm{int},|M|} = \frac{1}{2}\int_{-\infty}^{\infty} \Phi_{|M|}(t)\,\mathrm{d}t$ is the integrated relaxation time [25]. For each concentration p, we averaged the data over 16–32 configurations to obtain cumulants with an error of $(1\text{–}2) \times 10^{-2}$. As a typical example of the cumulant analysis, figure 1 shows the intersection of cumulants with a concentration $p = 0.8$ and linear sizes $L \in [20\text{–}60]$. In contrast to the two-dimensional Ising system which suffers from severe finite-size corrections (L-dependence of the intersection [24]) even for large lattices ($L \simeq 250$) [26], we find that these corrections are below our small statistical errors in three dimensions. For all concentrations we determined the critical temperatures $T_c(p)$ with a relative error $\Delta T_c/T_c \simeq 10^{-4}$ (table 1). This error was calculated from the variance of the intersection point using the whole set of cumulant data and its subsets. The critical temperature of the pure system is well known [27–29] and it is confirmed here with a small relative error of $\Delta T_c/T_c = 5 \times 10^{-5}$ using only a small amount of data. Our result for the concentration $p = 0.8$ agrees very well with the critical temperature $T_c(p = 0.8) = 3.4991(5)$ of Wang *et al* [30] who have determined T_c from the extrapolated susceptibility maximum.

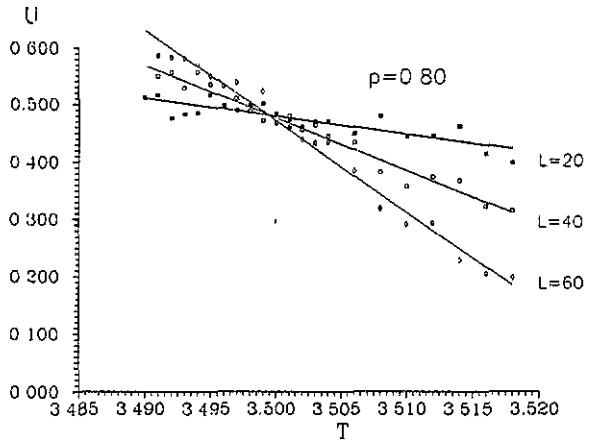

Figure 1. Cumulant U (1) of site-disordered Ising systems with a concentration $p = 0.8$. The critical temperature $T_c(p)$ has been determined from the intersection of $U(L, T)$. An average over up to 32 configurations for all temperatures and run lengths of $O(10^6)$ MCS/spin are necessary to reduce the error of U to $1\text{–}2 \times 10^{-2}$.

Table 1. Summary of the straightforward analysis of our finite-size data. Critical exponent ratios have been calculated by a fit of the data in the interval $L \in [20, 60]$ to their finite-size singularity. Exponents have been derived via the exponent relation (3) which permits one to obtain ν at the critical point T_c. The exponent α has been calculated from exponent relations.

p	T_c	β/ν	γ/ν	ζ/ν	
1.0	4.5115(1)	0.53(1)	1.95(2)	1.08(1)	
0.95	4.2622(4)	0.49(2)	2.00(3)	1.07(2)	
0.90	4.0108(5)	0.48(2)	2.02(3)	1.05(2)	
0.80	3.4992(5)	0.51(2)	1.98(3)	0.97(2)	
0.60	2.4220(6)	0.45(2)	2.09(3)	0.94(2)	
p	β	γ	ζ	ν	α
1.0	0.33(1)	1.22(2)	0.67(1)	0.624(10)	0.13(1)
0.95	0.31(2)	1.28(3)	0.68(2)	0.64(2)	0.08(3)
0.90	0.31(2)	1.31(3)	0.68(2)	0.65(2)	0.05(3)
0.80	0.35(2)	1.35(3)	0.66(2)	0.68(2)	−0.03(3)
0.60	0.33(2)	1.51(3)	0.67(2)	0.72(2)	−0.17(3)

Our finite-size simulations have been performed at the critical temperatures $T_c(p)$ determined above, measuring the usual magnetic and caloric properties [31]. In addition, we have investigated the magnetization–energy ($|\mathcal{M}|$–$\mathcal{E}$) correlation function

$$\Gamma T^2 = N\left(\langle|\mathcal{M}|\mathcal{E}\rangle - \langle|\mathcal{M}|\rangle\langle\mathcal{E}\rangle\right) \tag{2}$$

which is the temperature derivative of the spontaneous magnetization. $N = pL^3$ is the number of spins in the system. The finite-size divergence of Γ is described by the critical exponent

$$\zeta/\nu = 1/\nu - \beta/\nu \tag{3}$$

at the critical point [31].

We have carried out a very detailed error analysis which will be presented elsewhere [32]. The main source of statistical errors of thermodynamic observables results from the variance in configuration space which is considerably larger than the usual statistical errors from finite Monte Carlo sampling with typical run lengths of $1\text{–}3 \times 10^6$ MCS/spin. We have therefore averaged all data over several hundred configurations for each concentration [32] to reduce the configurational errors. In addition, we have calculated the possible systematic deviation of a thermodynamic observable from its true value at the true value of T_c which may result from the error of $T_c(p)$ as determined from the cumulant analysis above. The resulting total error is included in table 1, which summarizes our results for exponent ratios determined from usual finite-size scaling with lattice sizes $L \in [20, 60]$. From these exponent ratios, the exponents have been calculated via the exponent relation (3). We point out that this method of calculating the exponent ν requires only simulations at T_c.

The concentration dependence of measured exponents (table 1) apparently violates the expected universality of critical behaviour. However, it should be remembered that a crossover between the pure (P) and the weakly random (R) fixed point is expected from the renormalization group. In a finite-size scaling analysis this crossover leads to L- and p-dependent effective exponents [32]. The concentration dependence of the exponents (table 1) for $p \geqslant 0.8$ may be interpreted as a crossover between the pure and the random fixed point. But the large exponents γ and ν for $p = 0.6$ and $p = 0.5$ [32] exceed the difference between the pure and the random fixed point by a factor 3. Although the crossover between both fixed points has not been calculated explicitly, it is unreasonable to trace back such a large non-monotonous effect to a simple two-fixed-point crossover. We therefore conclude that the crossover in systems with strong disorder is more complex than expected.

We have analysed our simulational data with respect to the expected crossover between the pure and the random fixed point [1–3, 13, 15]. At both fixed points, the basic scaling exponents y_H^P and y_H^R of the magnetic field are equal within the reliability of Padè-approximants [15, 16]. Thus, $\gamma/\nu = 2y_H - d$ should not change remarkably with disorder. This expectation is satisfied within the errors by our results for low disorder (table 1), but it is not fulfilled at the concentration $p = 0.6$ which shows a definitely negative value of η. This is again an indication of a crossover phenomenon and it shows that the crossover behaviour of strongly disordered systems is not described just by fixed points P and R.

The basic thermal exponent y_t is more interesting since it has distinctly different values $y_t^P = 1.60$ and $y_t^R = 1.50$ at the fixed points [15, 16]. This permits a verification of both exponents from the simulation. We extracted the thermal exponent $y_t = 1/\nu$ by means of the function

$$\Upsilon \equiv \frac{1}{M} \left.\frac{\partial M}{\partial t}\right|_H = T_c(p) \frac{\Gamma}{M} . \tag{4}$$

It is easily verified from the finite-size scaling behaviour of M, that Υ depends only on y_t. The scaling function $L^{-y_t}\Upsilon(L)$ has been calculated from our data and it is plotted for all concentrations in scaling form (figure 2) with the exponents y_t^P for $p = 1.0$ and with y_t^R for $p < 1.0$. This figure contains the central result of this paper. It shows that disordered systems have a complex crossover before they converge to their asymptotic behaviour, which is consistent with the fixed point of weakly disordered Ising systems.

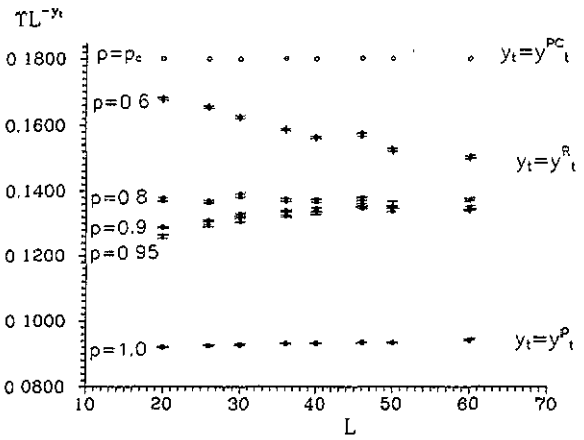

Figure 2. The scaling function $L^{-y_t}\Upsilon(L)$ is plotted as a function of system size L with the corresponding asymptotic exponents $y_t = y_t^{\mathrm{P}}(p = 1.0)$ and $y_t = y_t^{\mathrm{R}}$ $(p < 1.0)$. The figure shows that a complex crossover occurs in spin systems with general disorder. Statistical error bars of the scaling function are included. Small and large disorder leads to a different approach to the universal asymptotic behaviour. For interpretational purpose (see text), we have added the expected results of a future simulation slightly above the percolation concentration p_c, scaled with the percolation exponent $y_t = y_t^{\mathrm{PC}}$.

The pure system reaches its finite-size limit $L^{-y_t^{\mathrm{P}}}\Upsilon^{\mathrm{P}}(T = T_c, L \to \infty)$ already at low system sizes. Scaling corrections to asymptotic scaling are small and are therefore not visible within the resolution of figure 2. Disordered systems $(p \neq 1.0)$ approach a different asymptotic $(L \to \infty)$ value $L^{-y_t^{\mathrm{R}}}\Upsilon^{\mathrm{R}}$ $(T = T_c,\ L \to \infty)$. We stress that both values are universal since they are limits of a universal scaling function.

Figure 2 shows that the way disordered systems approach asymptotic behaviour depends very much on the degree of disorder. Weakly random systems $(p \geqslant 0.8)$ approach the asymptotic limit smoothly from below whereas strongly random systems $(p < 0.8)$ cross over from the opposite direction. In both cases, the asymptotic behaviour is reached at lattice sizes $L \geqslant L_c(p)$ with the length scale $L_c(p)$ depending on the concentration. We denote $L_c(p)$ the length scale of frozen disorder.

It is obviously not possible to make quantitive predictions about the functional p-dependence of $L_c(p)$. One can roughly estimate $L_c(p)$ to be about 50 for the weakly disordered systems with concentrations $p = 0.95$ and $p = 0.9$. The strongly random system with $p = 0.6$ does not really reach the asymptotic behaviour in our simulation up to $L = 60$, but the approach is nevertheless obvious in the scaling plot (figure 2). Rough extrapolation of $\Upsilon(L)$ for $p = 0.6$ to larger system sizes L leads to the expectation that the asymptotic behaviour is reached for $L \geqslant L_c \simeq 100$–$150$. We conclude that the length scale $L_c(p)$ strongly increases with dilution. Since the percolation fixed point becomes increasingly stable when the percolation concentration $p_c = 0.31$ is approached, the length scale $L_c(p)$ must diverge at p_c. Thus, we expect that a future simulation in the limit p_c^+ leads to the constant scaling function $L^{-y_t^{\mathrm{PC}}}\Upsilon(L)$ indicated in figure 2 by open symbols. Here, $y_t^{\mathrm{PC}} = 1/\nu^{\mathrm{PC}}$ is the thermal exponent of percolation [27]. The universal value of the scaling function in this limit remains to be determined.

Accidentally, the crossover function $L^{-y_t^R}\Upsilon(L)$ changes the sign of its derivative at a concentration $p \simeq 0.8$ so that the asymptotic range *appears* to be reached already for small system sizes. This effect explains why critical exponents of earlier Monte Carlo simulations [30,31] at this concentration showed up the theoretical exponents of the weakly random fixed point (R).

The crossover found in this work explains earlier reported simulational results [30,31] which apparently displayed non-universal behaviour of disordered systems. Experimental investigations of diluted magnets [33–34]† have also found concentration-dependent exponents which are now explained as a crossover phenomenon. We have shown that a simple two-fixed-point scenario is not the last word if general disorder is studied. While a simple crossover between the pure and the weakly random fixed point possibly accounts for the behaviour of systems above $p \simeq 0.8$, more strongly disordered systems necessitate a more refined analysis by an appropriate treatment of their percolative, i.e. structural effects which are relevant for non-asymptotic correlation lengths and system sizes, respectively. To this end, it is necessary to explicitly include the non-translational invariance of quenched disordered systems into theory. The corresponding operators have originally been eliminated self-consistently in the weak disorder theory [1]. Including them and taking additional frozen length scales $L_c(p)$ into account will lead to an interestingly higher complexity of the RG-analysis.

The influence of non-translational invariance of frozen disorder on the crossover is easily recognized from the qualitative behaviour of thermal and magnetic fluctuations in the crossover region [31,32]. The structural analysis of random configurations shows that there are large clusters of spins with a strong *intra*coupling. The *inter*coupling of these clusters is comparatively weak. This structure allows for large magnetic fluctuations and small energetic fluctuations in the region where the correlation length is smaller or comparable to the length scale of these configurational clusters. From this observation we expect that the length scale of frozen disorder $L_c(p)$ introduced above has a geometric interpretation in terms of geometrical clusters. However, a reasonable definition of clusters is a still a matter of discussion because is intimately related to the successful treatment of the subject.

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† We point out that the concentration dependence of measured exponents was not really admitted in many papers. Deviating exponents were often traced back to experimental and preparational problems with diluted samples. These objections are clearly ruled out by our Monte Carlo analysis.

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