Critical behavior of Ising models with static site dilution

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A Monte Carlo analysis of the ferromagnetic spin-$\frac{1}{2}$ Ising model with nearest-neighbor interactions and static (quenched) site dilution, where a fraction x, $0 \le x \le 0.2$, of the spins in a simple-cubic lattice are randomly replaced by vacant sites, reveals *effective* critical exponents varying continuously with x.

Dilute Ising models bear nowadays an undeniable interest both as a model of some physical situations one encounters in practice and as a well-defined arena to the analysis of the influence of disorder in critical phenomena,[1,2] i.e., any disorder (vacancies, incomplete strength of the interactions, etc.) randomly distributed throughout the Ising lattice may produce a new symmetry and, consequently, change the critical behavior originally shown by the pure system. It seems now that the behavior in the case of *annealed* vacancies or defects, which are characterized by having reached thermal equilibrium with the rest of the system, can be described by introducing a set of renormalized critical exponents.[3] The resulting critical behavior in the case of *quenched* (static) defects is, however, less understood at present. The exact results by McCoy and Wu,[1] allowing the strength of the (say) vertical interaction in the two-dimensional Ising model to vary randomly from row to row, have been the most important guide for experimentalists in that area. This particular kind of disorder produces the rounding of the original Onsager critical divergences, e.g., the resulting specific heat is differentiable at T_c, but it seems doubtful this is a general answer; for instance, the interactions proposed by McCoy and Wu reproduce a quasi-one-dimensional situation.[4] Approximate studies based on series expansions and renormalization-group methods can in principle be applied to more general situations, but it is difficult, so far, to evaluate their validity mainly because a richer structure of the critical point neighborhood makes those studies rather involved.[5−8] Nevertheless, plausible heuristic arguments by Harris[7] and some subsequent work[8] seem to suggest that the addition of vacancies to a system which undergoes a continuous transition would not affect the transition sharpness nor the corresponding critical exponents if the specific-heat exponent α of the pure system is negative; on the contrary, when $\alpha > 0$ (as for the three-dimensional Ising model) the critical behavior is expected to change. Most experiments on random systems seemed to reveal a pronounced rounding of the phase transition[9] though, more recently, sharp transitions and changing critical exponents have been reported[10,11] in agreement with the latest theoretical analysis of different disordered systems.[4,12,13]

Consequently, it seems that an accurate Monte Carlo analysis might be most helpful at the present time. In this paper we give some clear evidence of a second-order phase transition with effective critical exponents varying continuously for relatively small fractions of vacancies in a ferromagnetic Ising model studied by Monte Carlo methods. We expect to present soon a more complete description of the thermal and magnetic properties in our model;[14] see also Ref. 2 for a related effective-field treatment.

Our model and method are rather standard so that we refer elsewhere[14] for most details. The system Hamiltonian is defined as

$$H = -J \sum_{i,j}{}' s_i s_j , \qquad (1)$$

$J/k_B T_c = 0.221654$, where the sum extends over all nearest-neighbor pairs of sites in a simple-cubic lattice of size N with periodic boundary conditions; the disorder is introduced here by assuming $s_i = \pm 1$ except at xN randomly chosen sites where $s_i = 0$ $(0 \le x \le 0.2)$. Computations were actually performed on $N = 30^3$ and $N = 40^3$ lattices: no significant finite-size effects seem to affect our basic results. As a matter of fact, we know from our previous experience on Monte Carlo (MC) work that those sizes should produce asymptotic, $N \to \infty$, values for many purposes, and, for the x values considered here, different vacancy distributions produce, in practice, indistinguishable results. As compared to previous work basically referring to $N = 6^3$, 10^3, and 20^3 and $x \ge 0.2$,[15] our analysis here leads to definite conclusions concerning critical exponents because we consider larger N values and small fractions of vacancies, $x \le 0.2$, together with large samples of the equilibrium ensemble, more temperatures in the asymptotic regime $T \to T_c$ and perform a very detailed analysis of the data values. One should, in fact, be careful when considering disordered systems given the smallness of the expected effects and other inherent difficulties.[10,16,17]

Each equilibrium ensemble was generated by a Metropolis procedure: The $(1-x)N$ spins on the lattice are visited sequentially and flipped when $\Delta H \le 0$ or with probability $\exp(-\Delta H/k_B T)$ otherwise [ΔH is the change in the energy (1) which would produce the attempted flip]. An arbitrary starting configuration, generally obtained in a previous run at slightly lower and/or higher temperature, is allowed to evolve to reach equilibrium. The energy, $e \equiv \langle H \rangle /(1-x)N$, and the spontaneous magnetization,

$$m \equiv \frac{1}{(1-x)N} \left\langle \left| \sum_{i=1}^{N} s_i \right| \right\rangle , \qquad (2)$$

are then measured every time one completes from two to four visits to the whole lattice (depending on the value of $T - T_c$), thus practically avoiding correlations between successive measurements, and averaged typically over 5000—11 000 MC steps; larger "time" intervals were needed when extremely close to T_c. $\langle\ \rangle$ denotes our averaging procedure. Each series of values for e and m was continued until the corresponding distributions passed several Gaussianity tests; it became clear in this way that the consideration of an extra average over independent histories is rather irrelevant for this purpose. Note, however, that our data still suffers from typical errors, e.g., m presents finite-size effects very near T_c (so that the corresponding values are discarded for the present analysis), the system makes transitions between positive and negative magnetization states when extremely close to T_c (so that one has to analyze the m distributions with most care in those cases), and our values for the susceptibility and specific heat, obtained, respectively, from approximately Gaussian distributions for m and e by using the fluctuation theorem,[14] are always less reliable than the means m and e themselves.

The main overall conclusion is that the phase transition remains sharp for $x \leq 0.2$; for instance, the susceptibility-versus-temperature curves[14] present, at temperatures $T_c(x)$, a very pronounced peak, and we found no qualitative differences when comparing the cases $x=0$ and 0.2. Even more, the visual extrapolation of our data does not seem to support any rounding for larger x values, so that the smearing effects around $T_c(x)$ suggested by previous MC data[15] might be absent in much larger lattices.

The shifted critical temperature $T_c(x)$ decreases with increasing x; see Table I. Our values for $T_c(x)$ were obtained by looking for the best agreement between the specific-heat data and the numerical derivative of the energy, the latter obtained from a spline fit to the energy data. That is, we adjusted a family of cubic polynomials to the energy data, allowing for the known statistical errors, each polynomial connected to the following one at a knot where the function and its two first derivatives are required to be continuous. A few simple knots are located

along the T interval, in such a way that one obtains the best monotonous behavior of the second derivative at the knots, and a triple knot is located near the expected $T_c(x)$ in order to reproduce the specific-heat singularity. The location of the latter is then slightly moved until the differences between the resulting derivative and the raw data for the specific heat are minimized. Given that this procedure is very sensitive to the location of the triple knot, that it may just involve in practice the specific-heat raw data for $T > T_c(x)$, which is the one suffering from lesser errors, and that the energy data behaves quite well (e.g., our data for $x=0$ is practically indistinguishable from series results), our method should indeed produce reasonably accurate values for $T_c(x)$. These happen to be compatible with the values obtained by other procedures, namely we obtain practically the same values from the susceptibility divergence and from the short-range order parameter $\sigma = (N_{++})(N_{--})(N_{+-})^{-2}$ (where N_{++} represents the number of up-up pairs of spins in the system, etc.), which is observed to present a very well-defined cusp at T_c,[14] while our spline method allows us to reduce the error bars for $T_c(x)$.

A precise determination of $T_c(x)$ has indeed a great relevance when trying to compute critical exponents. For instance, β follows then from the relation $m\,(dm/dT)^{-1} = (T - T_c)\beta^{-1}$ which is very sensitive to the actual value of T_c. It becomes clear by analyzing the data after this equation that β increases with increasing x. In order to find a precise β_x, we fitted splines to the m data and looked for a T interval close to $T_c(x)$ giving the best coefficient of linear regression and minimizing the differences $\sum (m - B\epsilon^\beta)^2$; moreover, we still made minor adjustments of $T_c(x)$ at this step. Table I reports our values for β_x and $B(x)$; Fig. 1 depicts some graphical evidence. The same analysis can, in principle, be applied to

TABLE I. Change with x, the fraction of vacancies, of the critical temperature, magnetization exponent, and thermodynamic amplitude as obtained in the present Monte Carlo analysis. For comparison we also include the values (*) we obtain when the series results for $x=0$ and $0.967 < T/T_c \leq 0.989$, the critical region considered for the Monte Carlo data, are subjected to the same analysis.

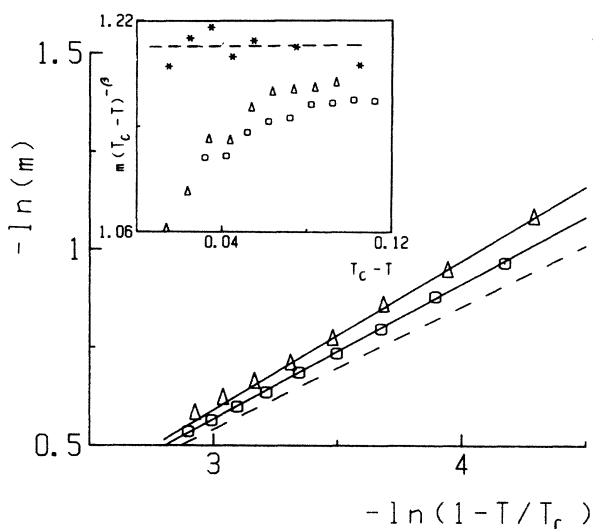| x	T_c	β	B
0	4.510±0.004	0.30 ±0.02	1.5 ±0.2
0.015	4.433±0.004	0.31 ±0.02	1.55±0.2
0.05	4.268±0.004	0.32 ±0.03	1.5 ±0.3
0.1	4.025±0.003	0.355±0.010	1.65±0.1
0.2	3.510±0.003	0.385±0.015	1.76±0.1
0*	4.510±0.002*	0.300±0.015*	1.5 ±0.1*

FIG. 1. Log-log plot of the spontaneous magnetization versus $1 - T/T_c(x)$ for $x=0.1$ (circles) and 0.2 (triangles). The dashed line is for $\beta=0.3125$; the solid lines are for $\beta=0.355$ and 0.385, respectively. The inset shows $m\,(T_c - T)^{-\beta}$ with $\beta=0.3125$ vs $T_c - T$; note that only our data for $x=0$ (asterisks) has a constant behavior.

our susceptibility values; while these data are much more noisy, so that we are unable to report reliable values for γ, it seems that γ increases with x in a way that, together with the scaling law $2-\alpha=\gamma+2\beta$, implies α going to zero or even becoming slightly negative in agreement with some recent experiments on random systems.[10] This, however, cannot be concluded directly from our specific-heat data.

Let us consider the simplest possible behaviors one may expect. If x is an *irrelevant* parameter, the critical exponents would be the same for all $x \neq 0$ as for $x=0$, and one should probably have[17]

$$\delta T_c \equiv [T_c - T_c(x)]/T_c = a_1 x + a_2 x^{2-\alpha} + \cdots \ ,$$

$$T_c \equiv T_c(x=0) \ .$$

This is not supported by our magnetization data nor by the values for $T_c(x)$ in Table I. If x is a *relevant* parameter, the critical exponents would take one value for $x=0$ and a distinct constant value for all $x \neq 0$, and probably[16] $\delta T_c = A x^{1/\phi}$, where ϕ is the crossover exponent describing the approach to the pure lattice behavior; the T_c data in Table I seem to support this scaling ansatz with $A \cong 1.06$ and $\phi \cong 1.01$ (these values differ from the ones given by Landau[15] where they are computed from an x range which is probably beyond the scaling regime). However, as evidenced for instance by Fig. 1, we are unable to detect any "impure" critical region very close to T_c leading to a β constant value for $x \neq 0$ different from our "ef-fective" values in Table I. It thus seems one should not exclude a third possibility in which there exists a line of fixed points, one for each x (so that, in particular, x is a *marginal* parameter), and the critical exponents vary continuously with x. Note thus that, although our data cannot exclude the existence of a tiny impure critical region which is practically unobservable for $0 < x \leq 0.2$, it was argued before[7] that the width of such a region should vary as $x^{1/\alpha}$ so that chances are that, even in the case it exists, it would be unobservable (before reaching the percolation threshold where the spontaneous magnetization vanishes), either experimentally or by Monte Carlo methods, and *effective* critical exponents varying continuously with x would always show up.

Finally, it seems interesting to note that it also follows from the above analysis that standard lattice sizes ($N \lesssim 10^5$) and statistics ($\sim 10^4$ Monte Carlo steps) can produce reasonable Gaussian distributions for the equilibrium values of the relevant magnitudes in disordered systems when the disorder only affects a fraction of the lattice sites within the limits considered here (i.e., $x \lesssim 0.2$). This fact should encourage new studies using Monte Carlo methods of disordered situations other than the vacancy dilution analyzed here. (We used in the present study around 150 hours of CPU time in an IBM 3083/XE01.)

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