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Monte Carlo Evidence for a Cusp in the Uniform Susceptibility of the Site-Diluted Simple Cubic Ising Antiferromagnet

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Monte Carlo simulations are performed for pure and site-diluted Ising antiferromagnets on a simple cubic lattice with up to 40^3 sites and impurity concentration $x = 0$, 0.2, and 0.5. For $x = 0.5$ a cusp emerges for the temperature dependence of the uniform susceptibility at the critical temperature which is contrasted with the smooth behavior for a pure antiferromagnet, in agreement with the theoretical prediction of Fishman and Aharony.

KEY WORDS: Critical phenomena; diluted Ising antiferromagnets; Monte Carlo simulation.

The study of critical phenomena in site-diluted Ising antiferromagnets is interesting from various viewpoints:

1. For magnetic field $H = 0$ the system represents a random-exchange Ising model. According to the Harris criterion,[1] a modification of the critical behavior due to the randomness of the system is expected (for a review of theoretical and experimental work see ref. 2). Furthermore, a nonmonotonic temperature dependence for the staggered susceptibility outside the critical regime is predicted.[3,4]

2. Even at $H = 0$ new effects for the uniform susceptibility have been predicted by Fishman and Aharony,[5] i.e., for the critical regime

$$k_B T\chi = A_1 + A_2 |t|^{1-\alpha} - A_3 |t|^{2\beta} \tag{1}$$

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with $t = (T - T_c)/T_c$. The last term is absent in pure antiferromagnets. It appears for $T < T_c$ and is related to the coupling between uniform and staggered thermal fluctuations. Because of $2\beta < 1 - \alpha$, it yields a stronger divergence of $d\chi/dT$ at T_c, i.e., a cusp emerges for the temperature dependence of the uniform susceptibility at T_c which is contrasted to the smoother behavior for a pure system. Such a peak has been found experimentally for two[6] and three[7,8] dimensions.

3. For $H \neq 0$ the system is a realization[5] of the random field Ising model; see, for instance, refs. 9 and 10.

Here we contribute mainly to the second point by reporting Monte Carlo results for the pure (impurity concentration $x = 0$) and the site-diluted Ising antiferromagnet ($x = 0.2, 0.5$) on a simple cubic lattice with 30^3 sites for $x = 0$ and 40^3 sites otherwise. The method is described in detail in ref. 2. We have performed 10^4 ($x = 0$), 1.5×10^4 ($x = 0.2$), and 2×10^4 ($x = 0.5$) Monte Carlo steps per spin, and have discarded the first 10%, respectively, to allow for relaxation to thermal equilibrium. For $x = 0.5$ our number of Monte Carlo steps per spin corresponds to about twice the number of steps used in the papers of Landau[11] and Marro *et al.*[12] for their investigation of the diluted simple cubic Ising ferromagnet. Furthermore, for $x = 0.5$ we have performed in addition a fully vectorized multi-spin Monte Carlo simulation for a 32^3 lattice with 10^5 Monte Carlo steps per spin, discarding the first 10^4 Monte Carlo steps per spin. The uniform susceptibility per site is calculated from the fluctuation-dissipation relation

$$k_B T \chi = \langle M^2 \rangle - \langle M \rangle^2 \tag{2}$$

with

$$M = \frac{1}{N} \sum_i S_i \xi_i \tag{3}$$

where $S_i = \pm 1$ represents the Ising variable, N is the number of sites, and the occupation number ξ_i has the value 1 (0) if site i is occupied by a magnetic (nonmagnetic) atom.

As shown in Fig. 1, there is evidence for the emergence of a peak for the temperature dependence of the uniform susceptibility in the highly diluted system ($x = 0.5$) which contrasts to the smoother behavior for $x = 0$. The behavior for $x = 0.2$ looks similar to that for $x = 0$ and is therefore omitted in Fig. 1. This is in agreement with the theoretical prediction,[5] with experimental results,[7,8] and with the expectation[13] that the amplitude of the peak is highest for $x = 0.5$, where statistical randomness is maximized. In the paper of Fishman and Aharony,[5] there is no quantitative estimation of the width of the temperature range where the coupling between uniform and staggered fluctuations should show up in a peak of the uniform susceptibility. However, it probably depends very strongly on the degree of statistical randomness, similar to the case of the random-exchange model,[1] so that the Monte Carlo simulations cannot resolve the possibly very narrow peak for $x = 0.2$. The evidence for a qualitatively different behavior of diluted and undiluted systems is further supported by the fact that the maximum of χ is located directly at $T_c = 1.85$ (in units of J/k_B) in the diluted system, whereas it is shifted to higher temperature for the pure case as predicted by Fisher and Sykes.[14] The

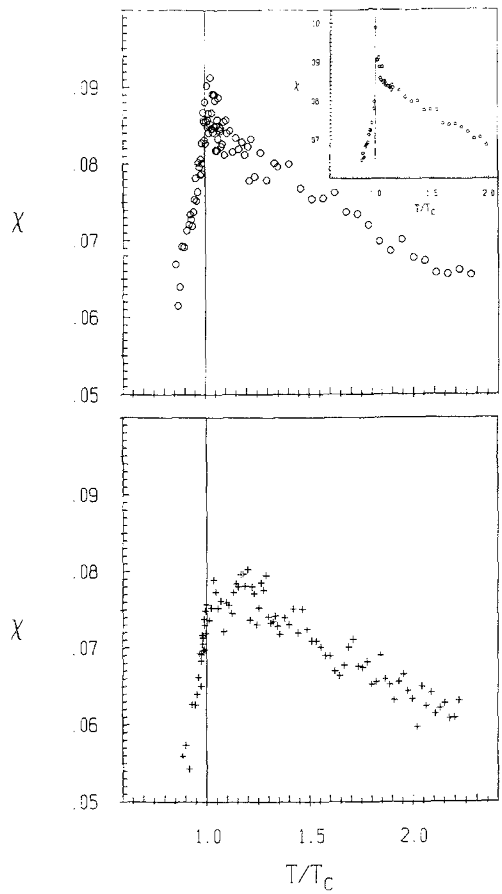

Fig. 1. The uniform susceptibility as a function of reduced temperature T/T_c for the site-diluted Ising antiferromagnet with impurity concentration $x = 0$ (crosses) and $x = 0.5$ (circles). The inset shows the data from the multi-spin Monte Carlo simulation.

critical temperature is determined from the Kouvel–Fisher analysis of the staggered magnetization, as described in ref. 2. We did not attempt to analyze the data quantitatively according to Eq. (1), because the statistical scatter very close to T_c is too large, even for the data from the multi-spin simulation.

We have also determined the critical exponent β of the staggered magnetization for $x=0$ and $x=0.2$. Because the simulation for the staggered magnetization of an antiferromagnet is totally equivalent to that for the uniform magnetization of a ferromagnet, the calculations for the ferromagnet from ref. 2 and for the antiferromagnet (present work) represent nothing but independent runs for the same problem. Accordingly, we obtain by a data analysis described in full detail in ref. 2 results which are equivalent within statistical error, i.e., $\beta = 0.291 \pm 0.03$ and $T_c = 4.508 \pm 0.009$ for $x=0$ (the corresponding results for the pure ferromagnet are[2] $\beta = 0.304 \pm 0.03$, $T_c = 4.513 \pm 0.009$) as well as $\beta = 0.364 \pm 0.03$ and $T_c = 3.510 \pm 0.007$ for $x=0.2$ (compared to $\beta = 0.392 \pm 0.03$, $T_c = 3.513 \pm 0.007$ for the diluted ferromagnetic model). Obviously the (probably effective) β value for the site-diluted model is again different from the value for the pure model, as predicted theoretically.[1]

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