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Critical Behavior of the Specific Heat for Pure and Site-Diluted Simple Cubic Ising Systems

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The exponent α of the specific heat C is determined for the pure and the site-diluted simple cubic Ising model (concentration $x = 0$, 0.2, 0.4 of nonmagnetic sites) by a finite-size scaling analysis of the peak value $C_{max}(L)$ for systems of linear dimensions $L = 8$, 16, 32, and 64. The C_{max} values are obtained by the Ferrenberg–Swendsen algorithm, using Monte Carlo data from a fully-vectorized multi-spin coding program. We obtain $\alpha = 0.11$ for $x = 0$ and a crossover to a negative α value upon dilution, with $\alpha = -0.029(4)$ both for $x = 0.2$ and $x = 0.4$.

KEY WORDS: Critical phenomena; diluted Ising model; Monte Carlo simulation; specific heat.

The critical behavior of spin systems with random structural disorder has been under debate for almost 20 years. It has been proved rigorously by Chayes *et al.*[1] that the correlation exponent ν for a very general class of disordered systems obeys the inequality $\nu \geqslant 2/d$, where d is the dimension of the system, yielding with the hyperscaling relation $\alpha = 2 - d\nu$ nonpositive values of α. This implies that the critical behavior of the 3D Ising model is modified by the introduction of structural disorder, because the specific heat exponent of the pure model is positive, $\alpha = 0.11$.[2]

Whereas it is thus well-established that α of the disordered 3D Ising model is nonpositive, no agreement has been found concerning the accurate value of α. Different field-theoretic renormalization calculations yield $\alpha = -0.013$,[2] $\alpha = -0.04$,[3] or $\alpha = -0.09$,[4] a recent Monte Carlo renormalization group study[5] obtains via the hyperscaling relation $\alpha = -0.064(13)$, and experiments[6] are consistent with $\alpha = -0.09(3)$. Conventional Monte Carlo studies on the specific heat suffer from the fact that α is very small and that the singular behavior is probably masked by

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nonsingular contributions or correction-to-scaling terms. As a result of the very small asymptotic critical temperature range for the specific heat, one must generate much highly accurate data very close to T_C for very large systems, which is aggravated by relaxation times increasing drastically with dilution. Therefore, Heuer[7] has calculated in his Monte Carlo study α not from the specific heat, but via the Rushbrook relation, yielding $\alpha = -0.16(4)$.

This paper represents an attempt to calculate α directly from Monte Carlo data for the specific heat C, for the diluted simple cubic nearest-neighbor Ising model (concentration $x = 0$, 0.2, and 0.4 of nonmagnetic sites). However, instead of analyzing the temperature dependence of C for a very narrow temperature range around T_C and a very big system, with all the uncertainties discussed above, we calculate the maximum (peak) $C_{\max}$ as a function of the system size (linear dimension L) and determine α from a finite-size scaling analysis. To obtain $C_{\max}$, we do not perform a conventional Monte Carlo simulation at various temperatures, but we apply the Ferrenberg–Swendsen algorithm[8] which allows one to calculate $C_{\max}$ very accurately from one Monte Carlo run at one temperature, if this temperature is close enough to the peak temperature $T_{\max}$ (see below).

The basic equation for the analysis is the finite-size scaling relation[9]

$$(C_{\max} - B) \sim L^{\alpha/\nu} \tag{1}$$

Because this relation holds strictly only asymptotically in the limit $L \to \infty$, we must consider rather large system sizes, and we have used $L = 8$, 16, 32, and 64. This requirement to have large systems in order to penetrate the asymptotic finite-size scaling regime replaces the necessity to consider temperatures very close to T_C in a conventional analysis of $C(T)$. The quantity ν is the critical exponent of the correlation length. For the pure system ($x = 0$) we insert $\nu = 0.63$,[2] whereas for the diluted systems a value of $\nu = 0.688$ is used as obtained by the Monte Carlo renormalization group calculation,[5] $\nu = 0.688(13)$. The constant B is an effective background coefficient[10] fitted so as to account approximately for the leading deviations from the asymptotic power law for $C(T)$. The value of B depends on the fitting details, for instance, on the temperature range used for the fit. Accordingly, various numbers are given in the literature for the pure model for fitting above (+) and below (−) T_C, $B_+ = -1.242$,[11] $B_+ = -1.6974$,[10] and $B_- = -1.965$.[10] We have performed the analysis for all these values of $B(x = 0)$ as well as tentatively also for $B = 0$. For the diluted system we insert

$$B(x) = B(x = 0)(1 - x) \tag{2}$$

with $B(x=0)$ given by the above-discussed values. At least for small dilution this ansatz seems to be justified, because in this case the energy per spin of the diluted system at the critical temperature of the diluted system is at least very close[5] to the energy per spin of the pure system at the critical temperature of the pure system.

To calculate the specific heat, we first made a good estimate for the temperature $T_{\max}$ where the maximum of the specific heat of the finite system is located. For the large systems ($L=32$, 64) we used the critical temperatures as obtained by the Monte Carlo renormalization group calculations,[5] for the small systems ($L=8$, 16) the peak temperature was determined approximately by a conventional Monte Carlo simulation. We then performed a long Monte Carlo run at this (already rather accurate) estimate $T^1_{\max}$ of the peak temperature, and calculated the probability distribution (histogram) $P(E, T^1_{\max})$ for the energy E of the system in zero field. With this probability distribution we can calculate the specific heat at $T^1_{\max}$ according to the fluctuation-dissipation relation. Furthermore, we can in principle evaluate from $P(E, T^1_{\max})$ according to ref. 8 the probability distribution $P(E, T)$ and hence $C(T)$ at any other temperature T, if we have determined with sufficient statistical accuracy $P(E, T^1_{\max})$ for all energies E, i.e., also for the long tails up to the maximum and the minimum possible energy of the respective system. In practice, this requirement represents a serious limitation of the method for large numbers of spins, where the probability distribution at a given temperature is very sharply peaked at the most probable value. Then there is only a small overlap of the probability distribution for temperatures which are not very close to each other, and due to the generally poor statistics for the tails of these probability distributions the original single-histogram Ferrenberg–Swendsen algorithm yields erroneous results as soon as one goes further away from the simulation temperature. One way to overcome this problem is to use multiple-histogram methods.[12] However, because we have already a very good estimate $T^1_{\max}$ for the peak temperature, it is sufficient to calculate $C(T)$ very close to $T^1_{\max}$ by the single-histogram method in order to find a more accurate estimate $T^2_{\max}$. The whole procedure is then repeated until the estimates $T^n_{\max}$ converge to the real peak temperature $T_{\max}$ (Table I). It turned out that for the big lattices ($L=32$, 64) the number n of iterations required was very small ($n=1$, 2 for the pure systems, $n=3$ for the diluted systems).

To evaluate the histograms, the fully-vectorized multi-spin coding progam described in ref. 13 has been applied. At each temperature we have performed at least 1.5×10^6 Monte Carlo steps per spin, omitting the first 5×10^5 steps for equilibration.

As a representative example, Fig. 1 shows the finite-size scaling plot

Table I. The Peak Temperature T_{max} and C_{max} for Various Concentrations x of Nonmagnetic Sites and Various Linear Dimensions L of the System[a]

	$L=8$	$L=16$	$L=32$	$L=64$
$x=0.0$				
T_{max}	4.028(3)	4.4560(1)	4.4915(1)	4.5060(1)
C_{max}	1.521	2.261	2.866	3.442
$x=0.2$				
T_{max}	3.2705(1)	3.4195(1)	3.4790(1)	3.4900(2)
C_{max}	1.051	1.358	1.551	1.475
$x=0.4$				
T_{max}	2.181(3)	2.3725(1)	2.3980(1)	2.4135(2)
C_{max}	0.541	0.686	0.787	0.738

[a] Values of T_{max} are in units of J/k_B, those of C_{max} in units of Nk_B.

for $B(x=0)=-1.6974$.[10] For the pure system, the finite-size scaling regime is penetrated already for $L \geqslant 16$. We obtain a positive slope of the plot according to a positive α, and for all nonzero values of $B(x=0)$ we find similar α values around 0.11 (Table II), in good agreement with the results of the field-theoretic renormalization.[2] It should be noted that this α value for the pure system yields, via the hyperscaling relation $\alpha=2-dv$, the correlation exponent $v=0.63$, in agreement with our above-assumed value. For diluted systems the slope changes from positive to negative with increasing L, indicating that the specific heat exponent is negative. In an earlier conventional Monte Carlo study of the site-diluted simple cubic Ising model[14] the system sizes $L \leqslant 20$ were too small to penetrate the asymptotic critical regime, and therefore this change of the slope for

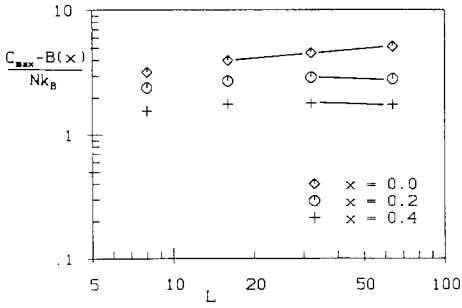

Fig. 1. Finite-size scaling plot for $C_{max}(L)$, assuming $B(x=0)=-1.6974$. Here $N=L^3$ denotes the total number of spins, and k_B is Boltzmann's constant.

Table II. The Specific Heat Exponent α for Various Concentrations x of Nonmagnetic Sites and Various Values of the Effective Background Coefficient $B_0 = B(x=0)$

	α			
x	$B_0 = 0$	$B_0 = -1.242$	$B_0 = -1.6974$	$B_0 = -1.965$
0.0	+0.166	+0.119	+0.108	+0.102
0.2	−0.049	−0.030	−0.026	−0.025
0.4	−0.065	−0.033	−0.028	−0.026

increasing L could not be observed. Assuming that we are in the scaling regime for $L \geqslant 32$ (which is of course not guaranteed and which could only be checked by very costly calculations for even larger lattices) we find the α values given in Table II. Within the uncertainties introduced, for instance, by the use of different effective background coefficients B (see above), we obtain for both concentrations $x = 0.2$ and $x = 0.4$ the same value of α, i.e., $\alpha = -0.029(4)$, which is closest to the value of $\alpha = -0.04$ obtained by the k-space renormalization calculation of Newman and Riedel.[4] From the hyperscaling relation we then obtain $\nu = 0.6763(13)$, consistent with the result $\nu = 0.688(13)$ from the Monte Carlo renormalization calculation[5] which we have used in Eq. (1) for the diluted system. Formally, our result for ν obtained from α seems to be considerably more accurate than the one from the Monte Carlo renormalization, which would give a rather large error limit for the exponent $\alpha = 2 - d\nu$, $\alpha = -0.064(39)$. However, one should take into account that our present result relies on the optimistic assumption that the scaling regime already has been reached for $L \geqslant 32$. Wang *et al.*[15] obtained for $x = 0.2$ and $L = 300$ by a single-cluster Monte Carlo algorithm the exponents $\gamma = 1.36 \pm 0.04$ and $\gamma/\nu = 2.00 \pm 0.01$, yielding $\nu = 0.680(17)$. This is consistent with the above-discussed results for ν, and gives an estimate for α (via the hyperscaling relation) of $\alpha = -0.04(5)$, which is, within the rather large error limits, again consistent with our α value and with the renormalization calculation of Newman and Riedel.[4]

To our knowledge this is the first time that the crossover from positive to negative α values upon dilution of the 3D Ising model could be demonstrated by Monte Carlo data for the specific heat.

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REFERENCES

1. J. T. Chayes, L. Chayes, D. S. Fischer, and T. Spencer, *Phys. Rev. Lett.* **57**:2999 (1986).
2. I. O. Mayer, *J. Phys. A* **22**:2815 (1989).
3. G. Jug, *Phys. Rev. B* **27**:609 (1983).
4. K. E. Newman and E. K. Riedel, *Phys. Rev. B* **25**:264 (1982).
5. T. Holey and M. Fähnle, *Phys. Rev. B* **41**:11709 (1990); M. Fähnle, T. Holey, U. Staaden, and P. Braun, *Festkörperprobleme: Advances in Solid State Physics*, Vol. 30, U. Rösler, ed. (Vieweg, Braunschweig, 1990), p. 425.
6. R. J. Birgenau, R. A. Cowley, G. Shirane, H. Yoshizawa, D. P. Belanger, A. R. King, and V. Jaccarino, *Phys. Rev. B* **27**:6747 (1983).
7. H.-O. Heuer, *Europhys. Lett.* **12**:551 (1990).
8. A. M. Ferrenberg and R. H. Swendsen, *Phys. Rev. Lett.* **61**:2635 (1988).
9. M. E. Fisher, in *Proceedings International Summer School "Enrico Fermi," Varenna, Italy, 1970*, M. S. Green, ed. (Academic, New York, 1971), pp. 1ff.
10. A. J. Liu and M. E. Fisher, *Physica A* **156**:35 (1989).
11. M. F. Sykes, J. L. Martin, and D. L. Hunter, *Proc. Phys. Soc.* **91**:671 (1967).
12. A. M. Ferrenberg and R. H. Swendsen, *Phys. Rev. Lett.* **63**:1195 (1989).
13. P. Braun, U. Staaden, T. Holey, and M. Fähnle, *Int. J. Mod. Phys. B* **3**:1343 (1989).
14. D. P. Landau, *Phys. Rev. B* **22**:2450 (1980).
15. J.-S. Wang, M. Wöhlert, H. Mühlenbein, and D. Chowdhury, *Physica A* **166**:173 (1990).