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THREE-DIMENSIONAL FERROMAGNETIC ISING MODELS WITH QUENCHED, RANDOM NON-MAGNETIC IMPURITIES*

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We investigate the thermal and magnetic properties of three-dimensional, ferromagnetic Ising models with quenched and random non-magnetic (site) impurities in the case of simple cubic lattices. The reported thermodynamic phase diagrams reveal in particular a sharp phase transition (e.g. in the magnetic susceptibility) for the (relatively small) impurity concentrations x considered here. We evaluate the critical temperature $T_c(x)$ and observe effective critical exponents varying continuously with x, probably corresponding to a crossover from pure to impure values. The latter, obtained here for $x = 0.2$, and the curve $T_c(x)$ are in good agreement with recent speculations. Our findings are also compared to some experimental data.

1. Introduction

Impure Ising models are recognized to bear a great theoretical interest in the analysis of the influence of disorder in critical phenomena. They also show a practical interest as a model of some familiar systems such as transition-metal oxides (which are usually found in Nature as $A_{1-x}O$), solid solutions with formula $A_{1-x}B_xC$ (where magnetic A atoms in the pure magnet AC are replaced by non-magnetic B impurities), etc. [1–5].

The substitutional disorder can in principle be *annealed* or *quenched*. In the case of *annealed* (site) disorder, the disorder variables on different sites are not independent but they have reached thermal equilibrium with the rest of the system, i.e. with the spin variables. This is not a very realistic situation given that the configurational disorder cannot be determined (or very rarely so) by magnetic interactions. This case is interesting mainly because of simplicity: the disorder variables can then be treated just as thermal variables and the system is reducible to the corresponding pure system. Concerning critical behavior, if the original (pure) specific-heat exponent α is positive (as for the three-dimensional Ising model of interest here), the annealed critical exponents are obtained from the pure ones as simple renormalizations which, in particular, imply that the specific heat presents no divergence [1, 6]. The case of *quenched* disorder, on the other hand, is characterized by a random distribution of disorder which remains frozen in time. That is, the disorder variables take a given equilibrium distribution at a temperature T' which is much larger (actually that randomness corresponds to $T' \to \infty$) than the temperature T for the equilibrium of the spin variables. Such a situation may be reached in practice after a quenched $T' \to T$ of the system in the case the disorder is inhibited from difussing by high potential barriers. It then follows that no reducibility to the pure system (like the one in the annealed case) applies now and that disorder and spin variables require very different treatments, e.g. the system free energy may be obtained in principle as an average over disorder configurations [2].

The critical behavior of quenched disordered systems remains a challenge for theoretical

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physicists which are still looking for definite answers to the most basic questions: Is the phase transition sharp or smeared? Is it first order or continuous? etc. In the case critical exponents exist, it may happen that they are the same as for the pure system, that a new set of critical exponents emerge, or even that one is faced with a much more complex situation. That is, the theory for quenched disordered systems is not quite clear-cut at present, mainly because there is a much richer (and more complex) structure in the neighborhood of the critical point than in the pure case, as we shall see later on. This is evidenced, for instance, by the fact that recent experiments give different (even qualitatively different) answers; e.g. most experiments on disordered systems seem to reveal a pronounced rounding of the phase transition [7] while other [8,5], following some theoretical trends [9, 10], report rather sharp transitions and changing critical exponents. There are also important experimental difficulties in this area; e.g. nonrandom distributions of disorder, which can seriously affect the system critical behavior, are unavoidable in practice [5].

The above situation immediately suggests that, as it was the case in some problems during the past, a Monte Carlo analysis might clarify somewhat the involved scenario, e.g. by excluding some of the possible issues. This goal turned out to be difficult in practice, however. This stems, for instance, from the pioneering works by Ching and Huber [11], Stoll and Schneider [12], Landau [15, 16] and others [13, 14]. Refs. 11–13 studied, almost simultaneously, quenched (and random) site-diluted two-dimensional Ising models to conclude that the exponents in this case ($\alpha = 0$) seem to equal the corresponding ones for the pure system. Their results, however, do not exclude the occurrence of a logarithmic singularity in the specific heat, and a relative smearing of the transition is reported; that work (dealing with up to 12 100 lattice sites) was prevented from more definite conclusions due to finite-size effects (which are "considerably stronger" than in pure systems). Refs. 14–16, on the other hand, deal with the three-dimensional case. Again the data, mostly corresponding to 20×20 simple cubic lattices (with the exception of an experiment in a $30 \times 30 \times 30$ system which is extremely diluted: 40%), is inconclusive for the same reason; e.g. the data show important variations for different impurity distributions.

We report in this paper the Monte Carlo analysis of three-dimensional ferromagnetic Ising models with quenched (and random) non-magnetic impurities. In order to avoid those problems, we investigated larger lattices (up to 64 000 lattice sites, which is practically the largest size we can handle in our computer) trying to minimize finite-size effects, we produced larger equilibrium ensembles to diminish the effect of the impurity distribution, and considered only small fractions of impure sites. We also considered more temperatures in the asymptotic, critical regime and performed a very detailed analysis of the data values. The resulting data is indeed reasonably well behaved; e.g. it recently allowed [17] to identify a change of the critical exponent for the magnetization with the fraction of impure sites. Here we extend the analysis in ref. 17 to describe the critical behavior of other magnitudes of interest such as especific heat and magnetic susceptibility. We also report on the system behavior far from the critical temperature and present thermodynamic phase diagrams. Our results are interpreted in the light of existing theory; they are also compared with some experimental data.

2. Description of the model

The model is defined through the Hamiltonian

$$H = -J \sum_{(i,j)}{}' s_i s_j , \qquad J > 0 , \tag{1}$$

where the sum extends over all nearest-neighbor pairs (i, j) of sites in a simple cubic lattice of size N with periodic (toroidal) boundary conditions, and $s_i = +1$, -1 or 0. Initially, the "occupation variables" s_i at xN randomly chosen sites are set $s_i = 0$ and the rest, $s_i = \pm 1$ (these values are also given at random). This simulates an infinite temperature state. The spin system (that is, the

set of spin variables capable of ± 1 values) is then let to evolve towards equilibrium at a given finite temperature T, while the "impurities" $s_i = 0$ remain frozen at their initial locations. The evolution is performed in practice by visiting sequentially the $(1-x)N$ spin variables on the lattice and flipping them, one after the other, according to the usual Metropolis algorithm. That is, one computes the change ΔH_i in the energy (1) which would cause flipping the spin at site i, and makes the flip $s_i \to -s_i$ when $\Delta H_i \leq 0$ or with probability $\exp(-\Delta H/k_B T)$ otherwise.

The magnitudes of interest are the energy, defined as

$$e = \langle H \rangle / (1-x)N , \tag{2}$$

and the spontaneous magnetization,

$$m = \frac{1}{(1-x)N} \left\langle \left| \sum_{i=1}^{N} s_i \right| \right\rangle , \tag{3}$$

where $\langle\ \rangle$ denotes an average of the corresponding quantities computed every time one completes several (up to six) visits to the whole lattice, thus practically avoiding correlations between successive measurements. The initial relaxation of the system was excluded from that average, until we were confident that the spin system was close to equilibrium; also, the average always included enough measurements to obtain distributions for H and $\Sigma_i s_i$ which succeeded to pass several gaussianity tests (this typically required more than 10^4 visits to the whole lattice). In addition to the quantities (2) and (3) we also computed the specific heat and magnetic susceptibilities from the respective mean squared fluctuations. Although these estimations do not behave so smoothly as the ones for e and m themselves, as we shall see see later on, it is noticeable that they agree reasonably well with the corresponding estimations obtained as temperature derivatives after making appropriate spline fits to the $e(t)$ and $m(T)$ data.

Our computations refer to $N = 30^3$ lattices for $x < 0.1$ and to $N = 40^3$ lattices for $x = 0.1, 0.2$. No significant finite size effects seem to affect our basic results, e.g. we checked that different impurity distributions produce in practice indistinguishable data for our choices of N and x. We also considered evolutions starting from an ordered state ($T = 0$). In order to minimize the computer time, however, we started sometimes the system evolution from arbitrary configurations, generally obtained in a previous run at slightly lower and/or higher temperature. In any case we found that the averages over independent histories, i.e. histories corresponding to different impurity distributions, could be avoided by considering larger equilibrium ensembles for a given random distribution.

3. Discussion of results

3.1. Energy

The behavior of the energy per magnetic ion, e, with T and x is illustrated by fig. 1. This reveals, both that the transition temperature decreases (approximately linearly) with increasing x and that, for any given temperature, $e(T, x)$

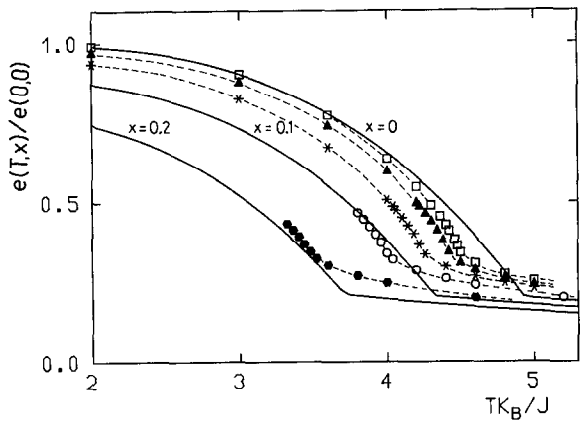

Fig. 1. System energy as defined in eq. (2), normalized to the minimum value $e(T=0) = -3$ for the pure ($x = 0$) case, versus temperature in units of k_B/J; see eq. (1). The symbols for the Monte Carlo data are as follows: squares □ ($x = 0$), triangles ▲ ($x = 0.015$), asterisks * ($x = 0.05$), empty circles ○ ($x = 0.1$) and full circles ● ($x = 0.2$). Typical error bars are considerably smaller than the size of the symbols used. The dashed lines are a guide to the eye except for $x = 0$ which corresponds to the series result for the infinite Ising model, ref. [18]. The solid line $x = 0$ is the Bethe-Peierls approximation to the pure case. The solid lines $x = 0.1$ and $x = 0.2$ are the result from a "cluster variation" computation in ref. 19.

also decreases with increasing x, the latter reflecting the fact that there is an "effective coordination" number $q = 6(1-x)$ (e.g. the zero field energy is $-3(1-x)J$).

The data in fig. 1 (which for the sake of clarity only includes a part of the available data) is compared with the series result for the infinite system in the case $x = 0$ [18] and with a "cluster variation" computation, which reduces to the Bethe–Peierls approximation as $x \to 0$, in the case $x \geq 0$ [19]. The former comparison shows up that, as expected, finite size effects are unobservable on this scale. The latter comparison confirms how the effective field theory developed in ref. 19 may be useful in some cases to interpret experimental data far from T_c.

A stringent comparison between the Monte Carlo data in fig. 1 and (real) experimental data can be obtained by considering the variation with x of the critical energy, or equivalently of the quantity $\langle s_i s_j \rangle$ per magnetic ion, say u, measured at T_c. By interpolating our data to T_c (as given below) we find approximately that

$$u(T_c, x) \equiv e(T_c, x)/e(0, x) \cong 0.328/(1-x) \qquad (4)$$

which is also consistent with previous Monte Carlo data [15, 16] for $x > 0.2$ (see fig. 2). Interesting enough, one has from series expansions [18] that $e(T_c, 0)/e(0, 0) = 0.328$ for the simple cubic lattice so that it follows from our result, eq. (4), that the minimum of $\langle s_i s_j \rangle$ the system needs to build up the magnetic ordered phase is a constant, independent of x (but probably depending on dimensionality and coordination number). The fact that the corrections to eq. (4), which is obtained here from rather small values of x ($x \leq 0.2$), are probably very small (if any) for larger x values follows apparently by noticing that the percolation threshold may be associated with $u(T_c) = 1$ which implies $x = 0.672$ in eq. (4): this is surprisingly close to the percolation value, $x_c \simeq 0.681$ for the present model.

The only related experimental values we have at hand are those in ref. 20 for the $Co_{1-x}Zn_xCs_3Cl_5$ compound which is a good example of Ising system with frozen-in non-magnetic impurities (Zn). The corresponding values for

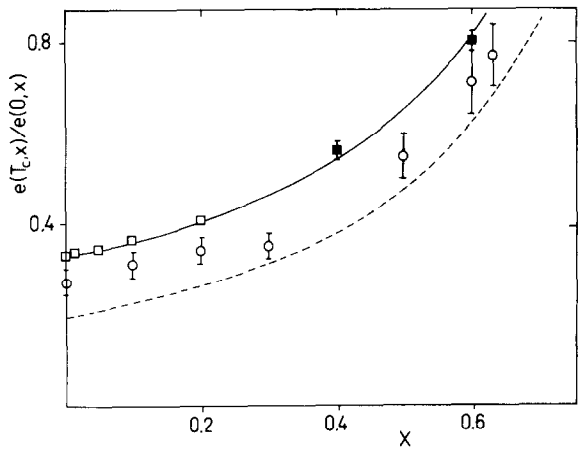

Fig. 2. The critical energy $e(T_c, x)$ divided by $e(0, x)$ versus x. The empty squares correspond to the present MC data, the full squares are the MC data in ref. 16, the circles represent the experimental data in ref. 20. The full line corresponds to $e(T_c, x)/e(0, x) = e(T_c, 0)/e(0, 0)\ (1-x)$ which implies that the minimum value of $\langle s_i s_j \rangle$ the system "needs" to build up the magnetic ordered phase is independent of x. The same qualitative result follows from the effective field treatment in ref. 19 which is represented here by a dashed line.

$e(T_c, x)$, which are obtained in this case from a numerical integration of the specific heat curves after making some necessary extrapolations for low and high temperatures, are shown in fig. 2. The agreement with the Monte Carlo data is reasonable having in mind that the experimental data is probably affected by larger error bars than suggested by fig. 2, e.g. due to the existence of microdomains and impurity gradients. In fact, it would be interesting to check the idealness of a given, real material sample against that property.

3.2. Magnetization

The behavior of the spontaneous magnetization with T and x is shown by fig. 3 where it is compared to the series result for $x = 0$ [18] and to an effective field theory [19] for $x \geq 0$. As expected, finite size effects are here small and controllable.

It seems noticeable the fact that, as $T \to 0$, the curves tend to a saturation value which is equal (or very close) to unity. This, however, cannot hold for larger x values [16, 19] because there is then some measurable probability for a spin to

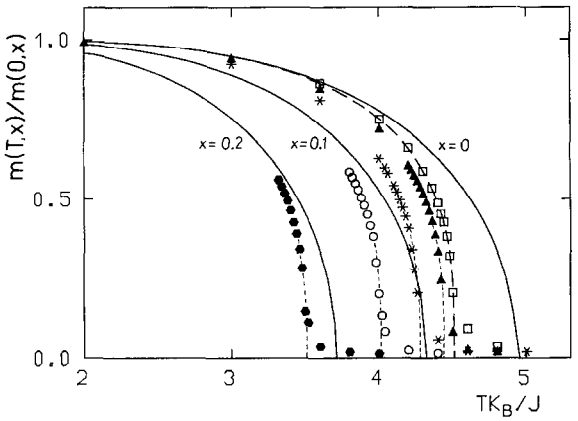

Fig. 3. Spontaneous magnetization normalized to its saturation value at zero temperature and $x = 0$. Same symbols as in fig. 1.

be completely surrounded by non-magnetic impurities. A straightforward estimation of this probability indicates that one should expect the bound $m(T=0, x) \leq 1 - x^6$.

3.3. Short ranged order

It turned out to be interesting to investigate the nature of the short ranged order as measured by the parameter

$$\sigma \equiv N^{++}N^{--}/(N^{+-})^2 , \tag{5}$$

where N^{++} represents the number of up–up pairs of spins in the system, etc. This actually measures the relation between ferromagnetic order and antiferromagnetic disorder in a given system state; it diverges as $T \to 0$ when $N^{+-} \to 0$, and $\sigma \to 0.25$ as $T \to \infty$. There easily follows a relation between σ, the energy and the magnetization in the case of randomly distributed impurities:

$$\sigma = \frac{(u+1)^2/4 - m^2}{(1-u)^2} , \tag{6}$$

where u represents $\langle s_i s_j \rangle$ per magnetic ion, that is $u = e(T, x)/e(0, x)$, as before.

For $x = 0$ the Bragg–Williams approximation leads to $\sigma = \frac{1}{4}$, independent of T, while the Bethe–Peirls approximation predicts a monotonous decrease of σ with increasing T, as shown by the solid line in fig. 4 [19]. The exact result by Onsager for the two-dimensional Ising model, on the other hand, implies a sharp singularity of σ at T_c, namely an infinite discontinuity of the derivative and $\sigma(T_c) = 8.49264$. In order to conclude about the corresponding behavior in three dimensions, we note that one has from eq. (6):

$$\frac{d\sigma}{dT} = (1-u)^{-3}\left[(1+u-2m^2)\frac{du}{dT} - 2m(1-u)\frac{dm}{dT}\right], \tag{7}$$

where one may convince by himself (trivially near T_c) that

$$(1+u-2m^2)\frac{du}{dT} \leq 0 , \qquad 2m(1-u)\frac{dm}{dT} \leq 0 . \tag{8}$$

That is, the sign of $d\sigma/dT$ depends on the term (8) which dominates in eq. (7) at a given temperature. At low temperatures one has $dm/dT \ll du/dT$ and σ increases with T; moreover, when m rapidly decreases as $T \to T_c$ it may happen that $d\sigma/dT$ changes sign. As a matter of fact, m and dm/dT become zero above T_c and σ decreases with increasing T. Therefore, one seems allowed to conclude on rather general grounds

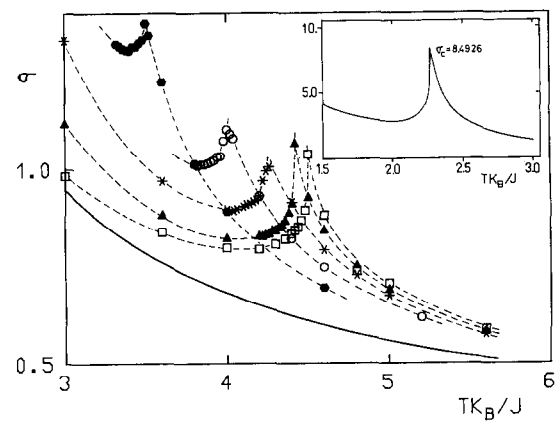

Fig. 4. The short ranged order parameter, as defined in eq. (5), as a function of T and x. Same symbols as in fig. 1. The solid line represents the Bethe–Peierls approximation for $x = 0$. The dashed lines are a guide to the eye. The inset shows σ in the case of the Onsager's exact solution for the pure two-dimensional model.

that in the case that $\sigma(T)$ presents any anomaly for the Ising model this will be located at T_c and will be associated to a change of sign of $d\sigma/dT$. One may reach the same conclusion by simply arguing qualitatively about the behavior of N^{++}, N^{--} and N^{+-} around T_c [21].

The MC results for $x = 0$ confirm indeed those expectations, as shown by fig. 4; as a matter of fact the observed behavior is very similar to the exact one in two dimensions. One may account for the small differences observed between those two cases (namely, the peak $\sigma(T_c)$ and the temperature region for which $\sigma(T)$ is an increasing function are smaller for $d = 3$ than for $d = 2$) by noticing that du/dT is proportional to the specific heat $C(\varepsilon)$, $\varepsilon \equiv 1 - T/T_c$, and that one may write

$$\frac{d\sigma}{dT} = \frac{2B^2\beta}{T_c}\,\varepsilon^{2\beta-1} - [1 + u - 2(B\varepsilon^{\beta})^2]AC(\varepsilon)\,, \tag{9}$$

where A and B are given parameters and β is the critical exponent for the spontaneous magnetization. The observed differences can thus be explained by using eq. (9) as a consequence, essentially, of the change of β with dimensionality [21]. What seems even more interesting for our purposes here is that the detailed analysis of the MC data for σ corresponding to different values of x (fig. 4) at the light of eqs. (6)–(9) allows the qualitative conclusion [21] that one should probably expect some change of β when x is increased from the pure value $x = 0$. We shall not describe here those details, which one may build up oneself from the above comments, because we expect to present some more conclusive evidences in the following. In any case, we note that the data in fig. 4 allows an easy evaluation of $T_c(x)$; the estimations for $T_c(x)$ obtained in this way are consistent with the ones in section 3.7 below.

3.4. Specific heat

The behavior of the specific heat with T and x is depicted by fig. 5. This is computed in practice as

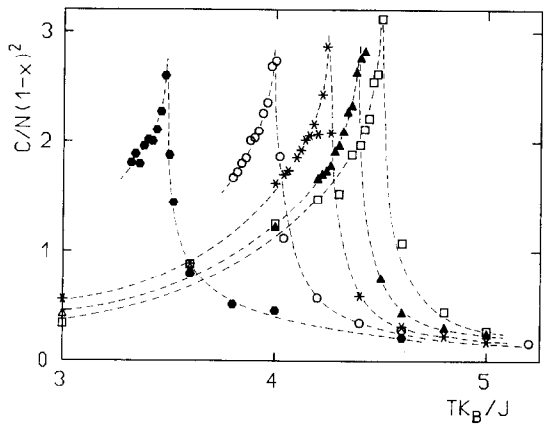

Fig. 5. Specific heat $C(T, x)$, as defined in eq. (10), per magnetic ion divided by $(1 - x)$; see the text for a comment on this normalization. Same symbols as in fig. 1.

$$C(T) = \frac{N(1-x)}{T^2 k_B^2}\,(\langle e^2\rangle - \langle e\rangle^2)\,. \tag{10}$$

We plotted in fig. 5, $C(T, x)$ per magnetic ion divided by $(1 - x)$ in order to account for the fact that the energy itself (not only its fluctuations) decreases with increasing x. The data is relatively scattered, as compared to the data in figs. 1–4, reflecting the fact that the relaxation time for fluctuations is much larger than the one for the means. Nevertheless, one may still recognize some general features of the data.

For instance, fig. 5 seems to suggest that the height of the observed peak is constant for $x > 0$ when one uses the proper normalization, i.e. a normalization consistent with the fact that there is an "effective coordination number" for the magnetic ions (section 3.1). That constancy of the peak is in contrast with the observation of decreasing height in the MC experiments reported in ref. 16; this probably indicates that the latter are certainly affected by finite size effects. One may also argue from fig. 5 that the height of the function for $x > 0$ is indeed finite in contrast with the expected divergence for $x = 0$; would that be the case, it would be consistent with $\alpha < 0$ for $x > 0$.

In order to strengthen this conclusion we also computed the specific heat as the temperature derivative of the energy by first making a spline fit to the data in fig. 1. The results for $x = 0$ and

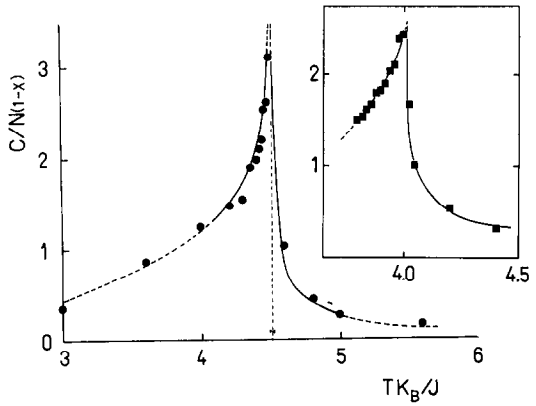

Fig. 6. The specific heat data in fig. 5 (full circles) is compared, in the case $x = 0$, to the result obtained after performing the temperature derivative of a spline fit to the energy data in fig. 1. The inset shows the corresponding case for $x = 0.1$.

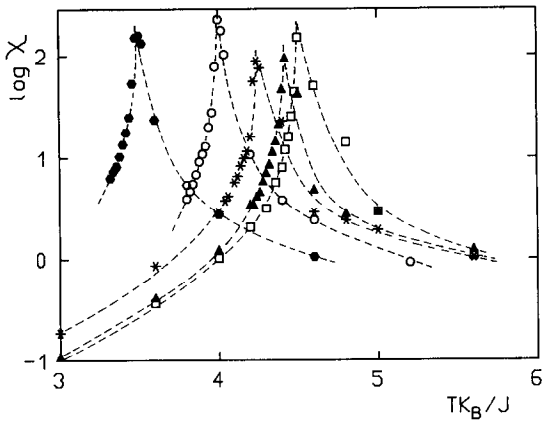

Fig. 7. Semilogarithmic plot of the magnetic susceptibility as defined in eq. (11). Same symbols as in fig. 1.

$x = 0.1$ are shown in fig. 6. This figure shows that both procedures to determine $C(T)$ are consistent with each other, implying the good quality of the data; note that one obtains in this way the expected divergence (dashed lines at the top of the figure) for $x = 0$. Fig. 6 also illustrates the fact that one may obtain a good value for T_c by this combination of the $e(T)$ and $C(T)$ data. The situation for $x > 0$ is very similar, except that the two branches of the temperature derivative seem then to intersect very early (fig. 6), in accordance with our comment in the preceding paragraph. We shall come later on to this fact which essentially agrees with recent theory [9, 10] and experimental observations [5]. This overall behavior, however, is basically different from the pronounced rounding which has been discussed frequently in the literature [3, 7, 20, 22, 23].

3.5. Magnetic susceptibility

Fig. 7 collects a part of the data corresponding to the magnetic susceptibility which is defined here, according to the fluctuation theorem, as

$$\chi = \frac{N(1-x)J}{k_B T} \left(\langle m^2 \rangle - \langle m \rangle^2 \right) . \qquad (11)$$

Note that this expression has no dimensions. The data is consistent with the situation described in previous setions; in particular, it follows strongly the suggestion that the phase transition remains sharp for the x values we consider here (as for the case $x = 0$) and, also, there is no evidence that this should not hold for larger x values.

3.6. Critical temperature

The data described before, namely figs. 1, 3–5 and 7, allow several independent estimations of $T_c(x)$. For instance, one may obtain directly rather good values for $T_c(x)$ from figs. 4, 5 and 7 which agree with each other. However, our aim in the next section (the computation of critical exponents) requires specially good values affected by the smallest error bars, and this compels one to be as precise as possible by trying to smooth out any oscillation of the data.

The energy data is very suitable for this purpose because it is specially well-behaved and corresponds to the mean value of the nearest-neighbor correlation which is practically unaffected by finite-size effects. Also, in order to enhance the discontinuity of the derivative of the energy at T_c, it turned out convenient to consider the quantity

$$e^* = (1-u)^2/(1+u)^2 , \qquad (12)$$

where $u = e(T, x)/e(0, x)$ as before. By fitting

cubic splines to those data points, identifying T_c with a sudden break in the slope of de^*/dT, and combining this information with the one which follows by similar methods from figs. 4 and 5 (see also fig. 6) we found the following tentative estimations (in units of k_B/J): $T_c(x=0)=4.510$, $T_c(x=0.015)=4.435$, $T_c(x=0.05)=4.270$, $T_c(x=0.1)=4.025$ and $T_c(x=0.2)=3.510$, where the errors are in the last digit. These values will be precised in the next section.

3.7. Critical exponents

The analysis of the critical behavior of impure systems has attracted much effort during the recent past. McCoy and Wu [3] succeeded in solving exactly the two-dimensional Ising model for a particular kind of disorder. However, more general situations require nowadays approximate methods, such as series expansions and renormalization group theory, whose range of validity is still an open question; in fact, a very rich structure near the critical point makes those studies difficult. The most popular finding in this area is perhaps the so-called Harris' criterion [24]; the general picture emerging from this and other efforts [1, 2] is as follows: The transition remains sharp for quenched disorder and a new fixed point becomes then stable, at least if the critical exponent characterizing the specific heat, α, is positive for the pure system (as in the three-dimensional Ising model of interest here) [28]. This seems to imply a new set of critical exponents for the impure system. When $\alpha<0$, on the contrary, the exponents should remain the same as for the pure case according to these studies (and a similar situation, perhaps with some "corrections to scaling", should probably hold for $\alpha=0$). Nevertheless, as indicated before in section 1, the experimental situation is not so clear-cut; also, the arguments leading to the above conclusions are not rigorous in general.

The data in the preceeding sections may in principle be of some help in this difficult area. To this end we note that the analysis of the data after the relation $m(dm/dT)^{-1}=(T-T_c)\beta^{-1}$ with $T_c(x)$ as given at the end of section 3.5 shows an apparent increase of β with x. In order to precise this fact, 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 squared differences $\Sigma(m-B\varepsilon^{\beta})^2$ where B represents the corresponding thermodynamic amplitude; also, we had to make minor adjustments of $T_c(x)$ at this step. We found in this way [17]:

$$T_c(x=0)=4.510, \qquad \beta_x=0.30, \tag{13a}$$

$$T_c(x=0.015)=4.433, \qquad \beta_x=0.31, \tag{13b}$$

$$T_c(x=0.05)=4.268, \qquad \beta_x=0.32, \tag{13c}$$

$$T_c(x=0.1)=4.025, \qquad \beta_x=0.355, \tag{13d}$$

$$T_c(x=0.2)=3.510, \qquad \beta_x=0.385, \tag{13e}$$

where T_c is in units of k_B/J, and $B(x)$ increases with x from $B(x)=1.5$ to $B(x)=1.76$; some graphical evidence of this fact was reported before [17]. Interesting enough, our method proves its consistency in the case $x=0$: we obtain precisely the values (13a) when the series results for the pure case [18] are subjected to the same analysis.

One may attempt an interpretation of the continuous variation of the measured β with x, (13), by considering the behavior of $T_c(x)$ near $x=0$. It is usually believed [25, 16] that having one value for the critical exponents when $x=0$ and a distinct constant value for all $x\neq 0$ (i.e. x being a relevant parameter in the terminology of the renormalization group theory) may be associated to the behavior $\delta T_c \equiv [T_c(0)-T_c(x)/T_c(0)] = Ax^{1/\phi}$ where ϕ represents the crossover exponent describing the approach to the pure system behavior. The data for T_c in (13) supports this scaling ansatz with $A=1.06\pm0.02$ and $\phi=1.01\pm0.01$. This suggests we are measuring in (13) an effective critical exponent, e.g. describing the approach from pure to impure behavior, the latter being represented by $\beta=0.38\pm0.02$, say. Would this be the case, one should expect an impure critical region, characterized by β-values between 0.30 and 0.38, whose width should increase with x, producing the ef-

fective behavior shown by (13). This impure region is not evident at all from the m data [17]; one may argue, however, that the data is not precise enough for this purpose. As a matter of fact, the width of such a region is expected to vary as $x^{1/\alpha}(\sim x^9$ in the present case) so that it would be unobservable here; even more, chances are that this region cannot be observed under any condition and that one should measure either impure values for β when x is large enough (say $x \gtrsim 0.2$) or effective values varying continuously with x when x is smaller. This is in good agreement (cf. (13)) with the experimental observation $\beta \simeq 0.35$ in $Mn_{0.86}Zn_{0.14}F_2$ [26] and with some recent computations on random Ising models [9, 10].

We are in favor of that interpretation of the observation (13). As a matter of fact, one should exclude the case that the critical exponents are the same for all $x \neq 0$ as for $x = 0$ (x being an irrelevant parameter) given the evidence (13) and also because one should probably then have $\delta T_c = a_1 x + a_2 x^{2-\alpha} + \cdots$ [27] which is not supported by the data. However, it is interesting to mention the case of a line of fixed points, one for each x, so that in particular x is a marginal parameter, and the critical exponents varying continuously with x. This is certainly very unlikely for our model here, but, to our knowledge, it has not been rigorously excluded by theory so far and it is compatible with the observation (13).

Some more evidence favoring x being a relevant parameter follows from the specific heat and magnetic susceptibility data as evidenced respectively by figs. 6 and 8. In fact, fig. 6 suggests, as discussed before, that α changes from positive to negative as x as increased from $x = 0$, and we are led to the same conclusion by analysing numerically the specific heat data after the method we applied before to the magnetization data; in the present case, however, the noise of the data prevents us from giving reliable estimations for α. Concerning the magnetic susceptibility data, on the other hand, fig. 8 suggests that γ also changes with x; again, we should only state this qualitatively. In any case, the observed variations on β, α and γ seem always roughly consistent with the scaling law $2 - \alpha = \gamma + 2\beta$.

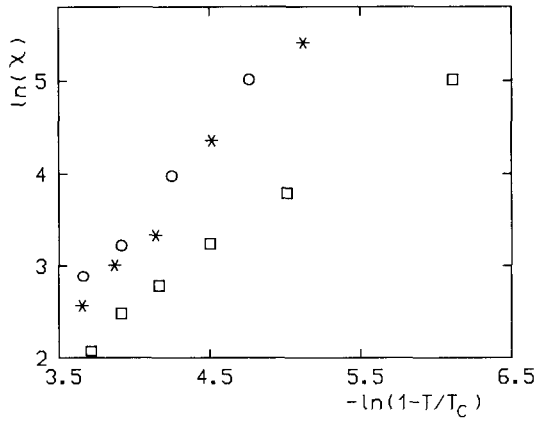

Fig. 8. Logarithmic plot of (a part of) the data in fig. 7 assuming the values (13) for $T_c(x)$. Same symbols as in fig. 1.

4. Conclusion

We described the relevant phase diagrams for the (quenched) impure, three-dimensional Ising model as a function of temperature and fraction of impure sites, x, in the case of relatively small values of x, $x \lesssim 0.2$. We also reported on other thermal and magnetic properties, including the behavior of specific heat, magnetic susceptibility and short ranged order parameter, and made comparisons with some available theory and experimental data. Our analysis clearly shows that the phase transition remains sharp in the sense that the magnetic susceptibility for the infinite system should diverge at $T_c(x)$; the specific heat critical exponents, however, change to negative for $x > 0$. Thus, there are new, impure values for α, β and γ which seem to satisfy the usual scaling law. The global evidence, on the other hand, is in favor of x being a relevant parameter, though it seems that effective critical exponents varying continuously with x will always be measured for $x \lesssim 0.2$ corresponding to a crossover towards the impure, fixed values. It should also be mentioned that our data cannot exclude definitely the (unlikely) case that the critical exponents actually vary continuously with x. That aim will require to consider larger values of x, much larger lattices and, most likely, special purpose computers.

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