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CONTINUOUS *VERSUS* FIRST ORDER TRANSITION IN DILUTE ISING ANTIFERROMAGNETS IN A FIELD

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Abstract. – A systematic Monte Carlo investigation of dilute Ising antiferromagnets in a uniform field as function of both dilution and ratio α of nnn to nn interactions on a cubic lattice is presented. A tricritical point is found in the range of dilution $0 \leq p \leq 0.3$ for a ratio $\alpha = -0.5$. Increasing p makes the first order region to shrink. On the other hand increasing α enlarges it. We present a new probabilistic mean field treament which yields the correct qualitative features of the phase diagram.

Random fields are obtained experimentally by applying a uniform field on dilute antiferromagnets [1]. Substitutional site disorder is the most usual experimental situation [2]. It is therefore of interest to obtain the phase diagram of site diluted Ising antiferromagnets in a field (DIAF). MC simulations of such systems in three dimensions with nearest neighbor (nn) interactions [3] suggested a continuous transition even for strong fields at a concentration $p = 0.3$ of non-magnetic sites. In contrast recent MC studies of the same model at a concentration $p = 0.2$ found a tricritical point by including next nearest neighbors (nnn) interactions for a ratio $\alpha - 0.5$ of nn to nnn interactions [4].

In this work we used MonteCarlo technique to obtain the phase diagram of DIAF. It appears to be non universal. Depending on the values of both dilution and the ratio α the transition from the disordered phase, as function of the field can be either always continuous, or first order with a tricritical point. A new probabilistic mean field theory which reproduces the qualitative features of Monte Carlo simulations is also presented.

We consider the following Hamiltonian

$$\mathcal{H} = J \sum_{\langle i,j \rangle} S_i S_j + \alpha J \sum_{\langle i,k \rangle} S_i S_k - H \sum_i S_i, \quad (1)$$

where $J > 0$ is taken as unit of energy in the following. H is the applied uniform magnetic field. The Ising spins S_i take the values ± 1 except at a concentration p of lattice sites where they are zero. These vacant sites are chosen at random. The first two terms in equation (1) are performed over all nn and nnn pairs respectively while the last one over all occupied lattice sites. We have carried out extensive MC simulations with different simple cubic lattice samples of size $N = 20^3$. Finite size effects have been studied for one case ($p = 0.2$, $\alpha = -0.5$) [4]. The periodic boundary conditions have been imposed throughout. The MC technique used here is the single-spin flipping procedure where in each run we discard a sufficient number of MC steps (MCS) per spin to equilibrate the system before averaging physical quantities over a number of MCS/spin. However there exist some difficulties in analysing MC data in first order transition [5]. Therefore the phase diagram shown in this paper should be read qualitatively. We now show our MC results. Details will be published elsewhere [6].

We show in figure 1 the phase diagram at $p = 0.1$, 0.2, and 0.3 for $\alpha = -0.5$ where results of Landau [7] for $p = 0$ are also presented. In the inset of figure 1 we show the tricritical temperature T_t as a function of p. It is observed that T_t decreases strongly with increasing p. This suggests that there exists a threshold p_c at which the tricritical point disappears.

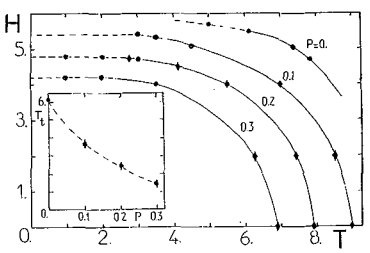

Fig. 1. – Phase diagram in the (T, H) plane for $\alpha = -0.5$ at various values of p. Results of runs with fixed H are denoted by solid circles and those with fixed T by diamonds. First and second order critical lines are shown by respectively discontinued and solid lines. Results at $p = 0$ are taken from reference [7]. The inset shows the tricritical temperature as a function of p.

We have also obtained the phase diagram in the (T, α) plane for $p = 0.2$ shown in figure 2. The tricritical temperature T_t decreases linearly with increasing α. We could not determine with accuracy the value of α for which the tricritical point disappears. This is due to the well known difficulty of MC simulation at very low temperatures. We think however that this value is close to -0.3. Note that the value $\alpha = -0.3$ is the

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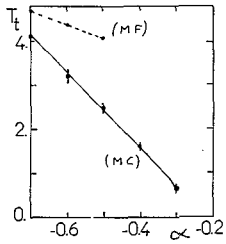

Fig. 2. – Tricritical temperature T_t *versus* α obtained by MC simulations at $p = 0.2$. Vertical bars indicate errors. The solid curve is a guide to the eye. Corresponding mean field tricritical temperatures are shown in dotted line.

critical value obtained from mean field theory for the disappearance of the tricritical point in the non-dilute case [8].

At this stage to discuss the above results we present a new mean field calculation [6]. Since mean field theory is a one-site approach, once dilution is introduced the various one-site configurations of the dilute problem should be included. There exist $7 \times 13 = 91$ configurations depending on the respective numbers n and l of both nn and nnn. We define these configurations through the variables $\gamma_{n,l}$ and $\delta_{n,l}$

$$\gamma_{n,l} = nJ + \alpha l J, \quad \delta_{n,l} = nJ - \alpha l J, \tag{2}$$

with the probability

$$p_{n,l} = \frac{c!}{n!\,(c-n)!}\frac{z!}{l!\,(z-l)!}\,(1-p)^{n+l}\,p^{c+z-n-l}. \tag{3}$$

The equations of state are thus averages of equations of state over the various configurations. We obtain

$$m = \sum_{n=0}^{c}\sum_{l=0}^{z} p_{n,l}\, m\left(\beta, H, m, m_s, \gamma_{n,l}, \delta_{n,l}\right), \tag{4}$$

and

$$m_s = \sum_{n=0}^{c}\sum_{l=0}^{z} p_{n,l}\, m_s\left(\beta, H, m, m_s, \gamma_{n,l}, \delta_{n,l}\right), \tag{5}$$

where formal expressions for $m(...)$ and $m_s(...)$ are taken from the pure case [8]. It should be noted that $m_s(\beta, H, m, m_s, \gamma_{0,0}, \delta_{0,0}) = 0$ due to the staggered symmetry of the problem. From equation (5) the Curie temperature at $H = 0$ is found to be $\beta_c = (p\gamma)^{-1}$, which is the correct mean field result. The values of tricritical temperatures obtained from equations (4) and (5) are shown in figure 3 as a function of dilution p. One notices a good qualitative agreement with MC results shown in the inset of figure 1. T_t as a function of α is shown in figure 2 (dotted line). The linear dependence of T_t on α is observed again here as in MC. Note however that for $\alpha \geq -0.4$ no solution is found and there is a discontinuity at $\alpha = -0.4$.

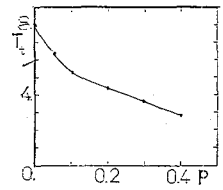

Fig. 3. – The critical temperature obtained by the probabilistic mean field equations is shown as a function of p at $\alpha = -0.5$.

In conclusion we have shown that phase diagrams obtained in experiments for various systems may exhibit quite different features. For a given experiment a tricritical point will thus be expected or not depending on the actual values of both p and α. We have also shown that results of MC simulations can be reproduced qualitatively by a very simple mean field model.

In order to compare our results to experimental situations one approach could be to select a particular physical system for which quantities like the coupling exchange energies for respectively nn and nnn interactions are known. The structure of the lattice is also of importance in the choice of the material since it defines the numbers of nn and nnn. On such a basis the corresponding theoretical phase diagram could be obtained and then compared to the experimental one.

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