MODEL STUDIES OF THE THERMAL AND MAGNETIC PROPERTIES IN DISORDERED SYSTEMS

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Ising models with quenched disorder have been studied, both by mean-field theory and Monte Carlo methods. The disorder is produced either by a magnetic field capable of values $+\infty$, $-\infty$ and 0, the value at each site given at random, or by non-magnetic impurities randomly distributed through the lattice sites.

1. The model

The basic model considered in our studies is the familiar spin-1/2 Ising model with isotropic nearest neighbor pair interactions defined by the Hamiltonian:

$$H = -J\sum_{i,j} s_i s_j, \tag{1}$$

where the sum runs over all nearest-neighbor pairs in a regular lattice with N sites and $s_i = \pm 1$. The disorder is introduced in the system by giving a fixed value s, independent of thermal fluctuations, to the spin variables located at xN lattice sites. The particular locations of the impurities are chosen at random. We consider the case (A) $s = \pm 1$, where the sign is also given at random, and (B) $s = 0$. This may be thought to correspond, respectively, to the action of a random strong magnetic field on a fraction of the magnetic ions and to the presence of quenched non-magnetic impurities. The model is, of course, an oversimplification of reality; it is expected however to shed some light on the study of the observed anomalies in some magnetic materials [1–8]

2. Mean-field treatment

The mean-field Bethe–Peierls method can be generalized to deal with cases A and B along lines reminding Kikuchi's cluster variation method [9,10]. To this end one considers all the different local spins configurations involving the first coordination shell on the assumptions: i) the different selected local configurations are independent of each other, ii) each local configuration is weighted by the corresponding probability and iii) the effect of the rest of the system enters through an internal mean field, the same one for every cluster. The resulting Hamiltonian may be written as:

$$-H/k_B T = \sum_{i=1}^{n}\left[hs_{oi} + (h+h')\sum_{j=1}^{q_i'} s_{ji} + K\sum_{j=1}^{q_i'} s_{oi}s_{ji} + (h+h')\sum_{j=1}^{n_i'} s_{ji} + K\sum_{j=1}^{n_i'} s_{oi}s_{ji}\right], \tag{2}$$

where s_{oi} is the central spin at each cluster, s_{ji} are the spins in the cluster sorrounding s_{oi}, h is proportional to the external field, n_i' is the number of sites affected by the disorder in the ith local cluster, and $q_i' = q - n_i'$ (q the coordination number). The sumation extends over all the n selected local clusters with $n = m_0 + \ldots + m_q$, where m_i is the number of different possible arrangements of the i-th configuration weighted by the corresponding probability. From the Hamiltonian (2) it easily follows that all the relevant physical magnitudes can be calculated by using averages in the form:

$$Q = \sum_{j=0}^{q} p_j Q_j, \tag{3}$$

where Q_j is the corresponding quantity obtained from a standar Bethe–Peierls treatment [11] for each local cluster, and p_j is the binomial probability.

In this way we have obtained analytical expressions for the magnetization, configurational energy, susceptibility and specific heat; the resulting behaviour is shown in figs. 1–4 where we compare cases A and B for selected values of the disorder concentration x.

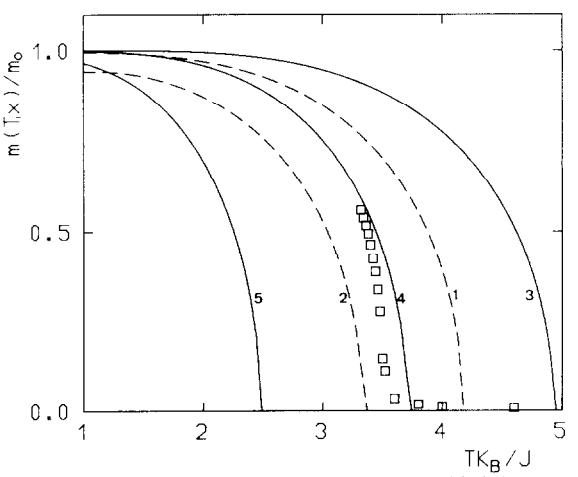

Fig. 1. Mean spontaneous magnetization devided by $(1-x)m(0,0)$, versus temperature for case A (broken lines 1 and 2: $x = 0.1$ and 0.2 respectively) and case B (solid lines 3, 4 and 5: $x = 0, 0.2, 0.4$), in the case of simple cubic lattice. The symbol corresponds to Monte Carlo results for a $40\times40\times40$ lattice, and $x = 0.2$ in case B.

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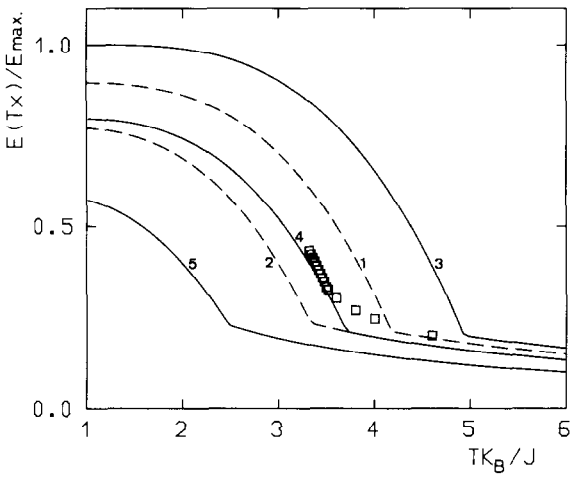

Fig. 2. The configurational energy of the system (sc lattice), divided by $(1-x)E(0,0)$, versus temperature at selected values of x; same symbols as in fig. 1.

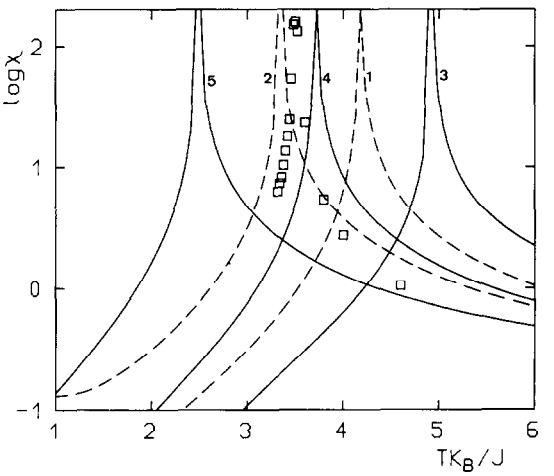

Fig. 4. Semilogarithmic plot of the magnetic susceptibility versus temperature. Same notation as in fig. 1.

Our mean field theory, also produces reasonable predictions for the variation of T_c with x. For instance in the case B, for a sc lattice we obtain:

$$T_c(x)/T_c(0) = \ln(3/2)/\ln\left(\frac{3-3x}{2-3x+x^6}\right) \qquad (4)$$

which agrees quite well with numerical and experimental data. The percolation threshold given by (4) is $x_c = 0.709$, which is very close to the series result ($x_c \approx 0.689$).

3. Monte Carlo simulations

Model B has also been studied by standard Monte Carlo methods [12] for small grade of disorder, $0 \leqslant x \leqslant 0.2$, in the case of a simple cubic lattice with N sites ($N = 27000$ and 64000), periodic boundary conditions and ferromagnetic nearest-neighbor interactions. Very large equilibrium ensembles were generated by the usual Metropolis dynamics. The configurational energy, e, and spontaneous magnetization, m, were computed from the equilibrium ensemble at each temperature T; the specific heat and magnetic susceptibility were then obtained from the dispersions of the m and e distributions, respectively, by fluctuations-dissipation theorems. Representative results are shown in figs. 1–4. A more complete account will be given elsewhere.

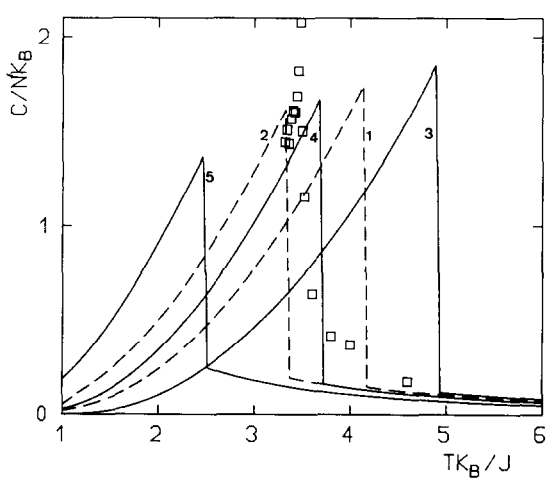

Fig. 3. Specific heat versus temperature for a sc lattice; $N' = (1-x)N$. Same notation as fig. 1.

4. Conclusions

We sketch here a very brief discussion and expect to report soon on the main conclusions of our work. The Monte Carlo analysis invólves a more detailed treatment of interactions and cooperative effects, our mean field treatments, however, seem to give a very reasonable semi-quantitative description of the numerical and experimental data. For example, our approach of case B allows a semi-quantitative description of the experimental data for any physical quantity over a broad range of temperatures and concentrations x, within a simple mathematic framework, and consequently, it should be useful in the analysis of experiments [10]. Concerning the critical behaviour of disorder systems, which is nowadays perhaps the most interesting point in this area, our mean field expressions only produce classical exponents, as one should probably expect. Nevertheless, there is a strong evidence that one may expect critical exponents varying with x in more realistic treatments. Namely, we observe that the "corrections to scaling" increase as x is increased. This result seems to hold for both models, A and B. The Monte Carlo analysis, on the other hand, clearly reveals effective critical exponents varying contynously with x within the range $0 \leqslant x \leqslant 0.2$. For example, the data reported in fig. 1 corresponding to $x = 0.2$, show a critical behaviour with $\beta = 0.385 \pm 0.015$ and $B = 1.76 \pm 0.1$, which clearly dif-

fer from the pure case values. The present work indicates a new basic interest to analyze these questions and, we hope, will stimulate further theoretical and experimental studies concerning disordered systems.

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