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FIRST VERSUS SECOND ORDER PHASE TRANSITION IN TYPE 1 ANTIFERROMAGNET ON THE FCC LATTICE

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Abstract. – We have used Monte Carlo simulations to investigate Ising systems on the FCC lattice with antiferromagnetic first neighbour interactions \( (J_1) \) and ferromagnetic second neighbour interactions \( (J_2) \) ("type 1 antiferromagnet"). Our results indicate that there is a first-order phase transition for \( J_2 / |J_1| \) up to at least as large as 1, a ratio four times as large as suggested by previous workers.

Antiferromagnetic order in an Ising system on the FCC lattice is characterized by frustration effects. We consider a system with both nearest and next-nearest-neighbour interactions, with the Hamiltonian

\[
H = -J_1 \sum_{\langle n,n \rangle} \sigma_i \sigma_j - J_2 \sum_{\langle n,n \rangle} \sigma_i \sigma_j.
\]

This system has three types of antiferromagnetic ground state, depending on the values of the exchange parameters \( J_1 \) and \( J_2 \), as shown in figure 1. The order parameter corresponding to Type 1, Type 2, and Type 3 antiferromagnetic order in the FCC lattice has, respectively, a number of components \( n = 3, 4, 6 \). In the latter two cases renormalization group arguments \([1]\) predict unequivocally that the transition will be first-order. On the other hand, in the Type 1 region \( J_1 < 0, J_2 = \alpha |J_1| > 0 \), the transition may be either first-order or second-order. It is this question which we address here.

![Diagram](image)

Fig. 1. – (a) The ground state phase diagram for the FCC Ising model; (b) One of the three degenerate AF1 states.

The most definitive previous study of this system, of which we are aware, is the Monte Carlo work of Phani, Lebowitz and Kalos [2]. These authors found that the transition, while clearly first-order for small \( \alpha \), apparently becomes second-order for \( \alpha > \alpha_c \approx 0.25 \). At first sight such a change in the order of the transition at an apparently arbitrary coupling constant ratio would seem surprising. An explanation has been proposed \([3]\), in terms of the more general phase diagram of the model in an external magnetic field \( H \). It is argued that a pair of triple points, which lie in the \( \pm H \) regions for small \( \alpha \), apparently coalesce at \( \alpha_c \) to a polycritical point at \( H = 0 \). This behaviour has apparently been confirmed by subsequent Monte Carlo work [4].

We were motivated to re-examine this question as a result of a study of random-field effects in diluted antiferromagnets which were yielding puzzling results. We have used standard "importance sampling" Monte Carlo simulations, for the case \( \alpha = 1 \), a point which previous work would suggest was well into the second-order region. We have studied lattices of size \( 4L^3 \) with \( L = 8, 12, 16, 20 \), i.e., up to 32,000 spins, with runs of typically \( 3 \times 10^4 \) MCS/spin. The quantities we have focussed on are the internal energy, not only its average value but also the nature of fluctuations, and on the order parameter.

For small values of \( \alpha \) we see hysteresis effects for all lattices sizes, and the transition is evidently first-order as expected. For \( \alpha = 1 \) there are no obvious hysteresis effects, and thus it might be concluded that the transition is indeed second-order. However a careful examination of the energy time-series, examples of which are shown in figure 2, suggests that this conclusion may be too hasty. For example, for the case \( L = 16 \) and \( T = 7.15 \) shown in figure 2, the fluctuations are clearly very asymmetric, suggesting perhaps the existence of two quasi-stable states with a small energy barrier between them. To pursue this further we have looked at the distribution of energies, in the form of histograms. For the small lattices, \( L = 8, 12 \), the distribution of energies becomes distinctively flat-topped near the apparent transition temperature, in contrast to the Gaussian distribution which would be expected for a second-order transition. For the larger lattices, \( L = 16, 20 \), the distribution develops a double-peaked structure. In figure 3 we show a comparison of energy distributions for different lattice sizes. The appearance of the double-peaked structure, and the fact that the peaks sharpen with increasing lattice size, is strongly suggestive of a first-order transition. In figure 4 we show a sequence of energy distributions for four different temperatures, for the case \( L = 20 \). It is
clear that the relative weights of the two peaks changes continuously with temperature, again as expected for a first-order transition.

These results would suggest that the transition at $\alpha = 1$ is first-order, albeit quite weakly so. This conclusion is thus in disagreement with previous work, which was restricted to smaller lattices and perhaps for this reason did not observe the double-peaked energy distribution. Interestingly our results, shown in figures 2 and 4, are qualitatively very similar to recent results [5] for the ten-state Potts model on the square lattice, which is known rigorously to have a first-order transition. This lends further credence to our conclusion for the present model. It is tempting to conjecture that the transition throughout the Type 1 region may be first-order, becoming second-order only at the limit $\alpha = \infty$ in which the lattice decouples to four independent ferromagnetic simple-cubic lattices.

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