A Simple Ferrimagnetic Ising Model

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A simple mixed-spin S = (1/2,1) Ising ferrimagnet on the square lattice is studied by low and high temperature series, and by Monte Carlo simulations. The former method indicates the presence of a tricritical point and consequent region of first-order transitions, while no evidence for this is found from Monte Carlo studies. A possible explanation is that the transition is very weakly first order.

1. Introduction

Ferrimagnets are materials where different sublattices have opposing magnetic moments of unequal magnitude. Thus, unlike antiferromagnets, these materials have a net moment at low temperatures which vanishes at a critical temperature T_c. In addition, since the sublattice moments will, in general, have a different temperature dependence, there is the possibility that they may exactly cancel at some lower temperature T_{comp}, known as a **compensation point.**

Studies of ferrimagnetism in quantum models have, to date, generally used mean-field approaches, which are of questionable validity. Consequently there has been much work, in recent years, on simpler mixed-spin Ising ferrimagnets where exact or numerically accurate treatments are possible. Such a model is studied in the present work. The model, shown in Figure 1, is a bipartite square lattice with S=1/2 spins on one sublattice (A) and S=1 spins on the other (B), with nearest-neighbour interactions and a single-ion anisotropy term at the S=1 sites. The Hamiltonian is

$$H = J \sum_{<ij>} \Sigma\, \sigma_i\, S_j - D \sum_i S_i^2$$

A schematic phase diagram is also shown in Figure 1. For D/J > -4 there is a transition line separating the low-temperature ferrimagnetic phase from a high-temperature paramagnetic phase. At D/J = -4 the ferrimagnetic and S=0 ground states are degenerate, and for D/J < -4 the ground state is infinitely degenerate with no magnetic order.

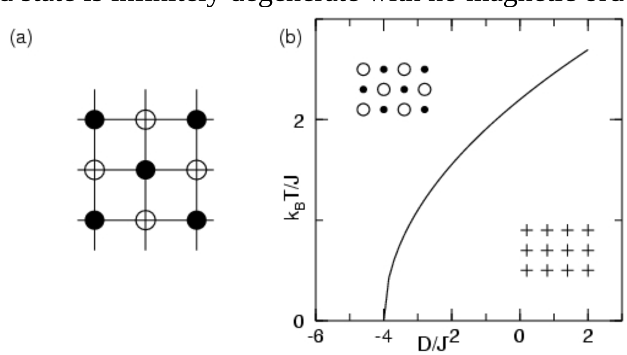

Fig. 1. The ferrimagnetic model(a), and a schematic phase diagram(b).

The mean-field phase diagram was obtained by Kaneyoshi and Chen [1], who found a compensation point for -4 < D/J < -2 ln 6 (-3.3535...). In addition they found a **tricritical point** at D/J = -3.720, and thus a first-order transition for -4 < D/J < -3.720. A more recent, and more reliable study, using Monte Carlo and transfer matrix methods, found neither a compensation point nor a tricritical point [2].

Because of this disagreement it seemed worthwhile to study the model by another systematic approach, that of high- and low-temperature series expansions. Our result [3], to be discussed below, found no compensation point, in agreement with [2], but did find a signature of a tricritical point near D/J = -3.1. We have subsequently carried out Monte Carlo studies at D/J = -3.6, where the series clearly indicate a first-order transition. These results are presented here for the first time. Surprisingly, no indication of a first-order transition is found.

2. Series Expansions

Series expansions have, in the past, been used successfully to identify and locate first-order transitions, by matching the free energies obtained from expansions in the high- and low-temperature phases. For a second-order transition the curves should meet smoothly, while a discontinuity in slope is an indication of a first-order transition.

Our series [3] are expressed in the form

$$-\beta f_{HT} = \tfrac{1}{2}\ln 2/(1-p) + \sum_{r=2}^{\infty} A_r(p)K^r$$

$$-\beta f_{LT} = 4\beta J + \beta D + \sum_{r=2}^{\infty} \Psi_r(y)u^r$$

where $K = J/k_BT$ and $u = e^{-2K}$ are the usual high- and low-temperature expansion variables, $A_r(p)$ and $\Psi_r(y)$ are polynomials, which have been computed to orders 16 and 19 respectively, and $y = e^{-\beta D}$, $p = 2/(2+y)$.

Figure 2 shows the free energy matching procedure for various D/J. It is apparent that for D/J > -3.0 the curves meet smoothly, whereas for D/J < -3.0 there is a clear discontinuity in slope, indicating a first-order transition.

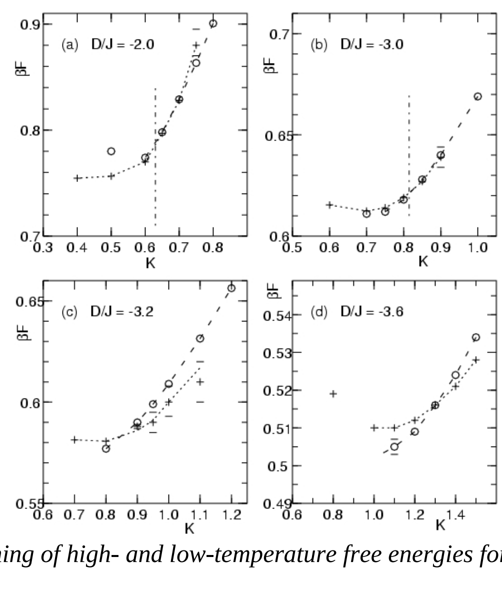

*Fig. 2. Matching of high- and low-temperature free energies for various **D/J**.*

3. Monte Carlo Simulation

In view of the discrepancy between the Monte Carlo results of [2] and our series results [3], we have carried out further Monte Carlo studies, but using the Wang-Landau method [4]. This new method is not based on Metropolis importance sampling at particular temperatures, but obtains the density of states $\rho(E)$ directly. The canonical distribution $P(E) = \rho(E)\exp(-E/k_BT)$ can then be obtained at any temperature, and used to compute all of the thermodynamic quantities.

We have adapted the algorithm to the present problem, and obtained the density of states for L x L lattices with L=16,24,32,48. Figure 3 shows the specific heat as a function of temperature for the four lattices for the case D/J = -3.6.

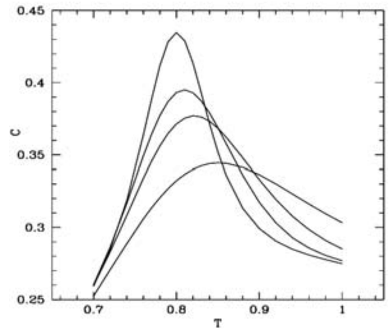

Fig. 3. Specific heat versus temperature for L x L lattices with L=16,24,32,48.

As is apparent, the specific heat peak sharpens, increases in height, and moves to lower temperatures for increasing L. This is, however, characteristic of both second- and first-order transitions, noting that a weak first-order transition can be difficult to distinguish from a true second-order transition.

The canonical probability P(E) is potentially a better discriminator of the order of the transition. For strongly first-order transitions P(E) should be double peaked at and near the transition temperature. In Figure 4 we show P(E) for the largest lattice studied, 48 x 48, at T=0.795, the temperature of the specific heat peak. There is clearly no double peak.

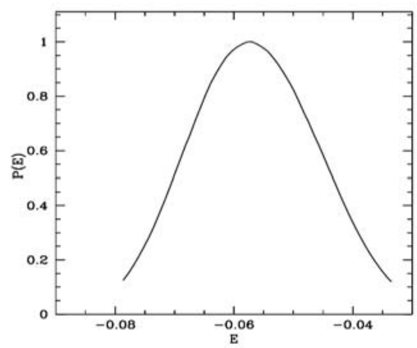

Fig. 4. Canonical probability versus energy for L = 48 at the temperature of the specific heat peak.

4. Conclusions

The series work and early and subsequent Monte Carlo studies continue to give conflicting results for the existence of a tricritical point and consequent region of first-order transitions in this simple model. A possible explanation is that the transition is very weakly first-order, and thus difficult to distinguish from a continuous transition. The puzzle remains!

Acknowledgments

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