Ferrimagnetism and Compensation Points
in a Decorated 3D Ising Model

J. Oitmaa and Weihong Zheng

[a] *School of Physics, The University of New South Wales, Sydney, NSW 2052, Australia.*

We give a precise numerical solution for a mixed-spin Ising model with $S = \frac{1}{2}$ on the sites of a simple cubic lattice and $S = 1$ spins on the nearest neighbour bonds. The solution shows the existence of ferrimagnetism, compensation points, and reentrant behaviour.

Ferrimagnets are materials where ions on different sublattices have opposing magnetic moments which do not exactly cancel even at zero temperature. [1] An intriguing possibility then is the existence of a compensation point, below the Curie temperature, where the net moment changes sign. This has obvious technological significance.

There has been considerable work in recent years in studying these phenomena through simple models [2-7], where treatments beyond mean-field theory are possible. Of particular interest are decorated systems, which can be mapped exactly onto simpler models, and in this way solved either exactly or to a high degree of numerical precision.

We consider a simple cubic lattice with N spins $S_A = \frac{1}{2}$ on the vertices and $3N$ spins $S_B = 1$ decorating the bonds. The model and its interactions are shown in Figure 1. The Hamiltonian is taken as

$$H = J\sum_{<ij>}\sigma_i S_j - J'\sum_{<kl>}\sigma_k\sigma_l - \Delta\sum_i S_i^2 \quad (1)$$

where $\sigma_i = \pm\frac{1}{2}$, S_j = -1, 0, 1. The terms in H represent, respectively, antiferromagnetic exchange between neighboring $S = \frac{1}{2}$, $S = 1$ spins, ferromagnetic exchange between nearest $S = \frac{1}{2}$ spins, and a single ion anisotropy on $S = 1$ sites.

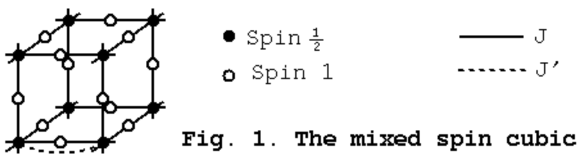

Fig. 1. The mixed spin cubic lattice.

Dakhama [6] has considered a similar model on the square lattice, and obtained an exact solution confirming the existence of compensation points. Our calculation is a generalization of this work.

The basic idea is to take a partial trace over the S spins, transforming the model to a spin-$\frac{1}{2}$ Ising ferromagnet on a simple cubic lattice, with coupling constant

$$\widetilde{K} = K' + 2\ln(\Sigma_1/\Sigma_2) \quad (2)$$

with

$$\Sigma_1 = 1 + 2e^D\cosh K, \quad \Sigma_2 = 1 + 2e^D \quad (3)$$

and with $K = \beta J$, $K' = \beta J'$, $D = \beta\Delta$, $\beta = 1/kT$.

The critical point of the nearest neighbour spin-$\frac{1}{2}$ Ising model on the simple cubic lattice is known to high accuracy as $\widetilde{K}_c = 0.88664$, [8] and hence our model has a critical line, which can be expressed, for $S = 1$, as

$$e^{K'/2}(1 + 2e^D\cosh K) = 1.5580(1 + 2e^D) \quad (4)$$

The spontaneous magnetizations of the two sublattices are easily obtained as

$$\langle\sigma\rangle = \tfrac{1}{2} M_0(\widetilde{K}), \quad \langle S\rangle = 2\gamma\langle\sigma\rangle$$

where $M_0(K)$ is the magnetization of the spin-$\frac{1}{2}$ Ising model on the simple cubic lattice, which is known numerically to high accuracy, and $\gamma = \Sigma_3 / \Sigma_1$, with $\Sigma_3 = 2e^D \sinh K$. The total magnetization is then given by

$$M / N = \langle\sigma\rangle - 3\langle S\rangle = (1 - 6\gamma)\langle\sigma\rangle \quad (5)$$

and hence any compensation point must lie on the line $6\gamma = 1$. Explicitly, for S = 1, the compensation point line is

$$12e^D \sinh K = 1 + 2e^D \cosh K \qquad (6)$$

Equations (4) and (6) are then solved numerically. The results are exact, to within the very small numerical uncertainity in $\widetilde{K}_c$.

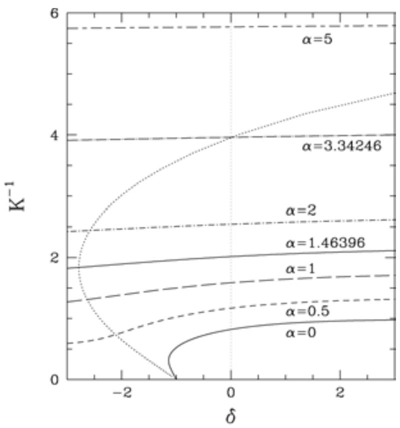

Fig. 2. The phase diagram of the mixed spin cubic lattice. Lines give critical temperature versus single ion anisotropy for various strengths α of the second-neighbour interaction. The dotted line is the compensation point line (Eq. 6).

Figure 2 shows critical lines in the $K^{-1} - \delta$ plane ($\delta = D / K$) for various values of $\alpha = K' / K$. We see, as expected, that increasing the second-neighbor coupling increases the critical temperature as does increasing the anisotropy parameter Δ. The critical line for α=0 shows reentrant behaviour, i.e. two phase transitions, for a small range -1.14046 < δ < -1.0. At very low temperatures the system will be disordered, since Δ < 0 favors the state S=0 at B sites. As the temperature increases the system orders at a lower critical temperature T_{C_1}, passes through an ordered phase, and then disorders again at an upper critical temperature T_{C_2}. Any nonzero second neighbor interaction will give rise to ordering at T = 0 and at low temperatures, and hence there will be a single critical point (subject to the caveat below). Reentrant behaviour of this kind was found in the approximate treatment of the square lattice [5], but was shown to be spurious by the exact solution [6]. For the simple cubic lattice it is a real effect.

The compensation point line is shown in Figure 2 as a dotted line. If this line lies below the phase transition line a compensation point will be present. Thus for α = 0 these is no compensation point, i.e. a second-neighbour interaction is essential. For δ < -2.7858 no compensation point is possible, while for -2.7858 < δ < -1 two compensation points will occur for sufficiently large α. For δ > -1 a single compensation point will occur for sufficiently large α.

Careful analysis of Eq. 4 for small α reveals even more interesting behaviour. In Figure 3 we show critical temperature curves in the vicinity of δ = -1 for several α values. As is seen, for 0 < α < 0.1087 the curve is S-shaped, and hence the system has three critical points, going from an ordered state to a disordered state, then back to an ordered state and eventually to a high-temperature disordered state. While such behaviour has been seen before in approximate treatments, as for example in the square lattice by Kaneyoshi [5], we are unware of any cases where it has been demonstrated in an exact treatment.

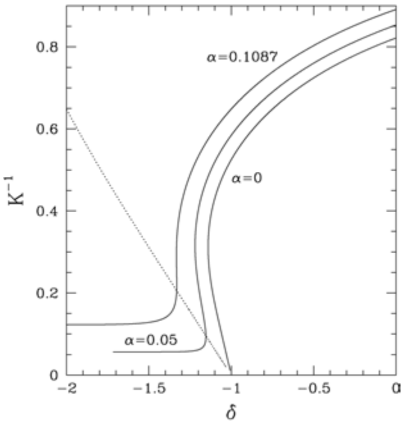

Fig. 3. Critical temperature versus anisotropy for small α. In the range 0 < α < 0.1087 the system will have three critical points. The dotted line is the compensation point line (Eq. 4).

It is instructive to compute the total magnetization as a function of temperature, for particular (α, δ), to display some of the features discussed above. In Figure 4(a) we show magnetization versus temperature for the case α = 3.2, δ = -2.5. The two compensation points are evident. Figure 4(b) shows magnetization versus temperature for α = 0.05, δ = -1.2. This case has three critical points. The compensation point line falls in the intermediate disordered phase, and hence there is no compensation point for this case.

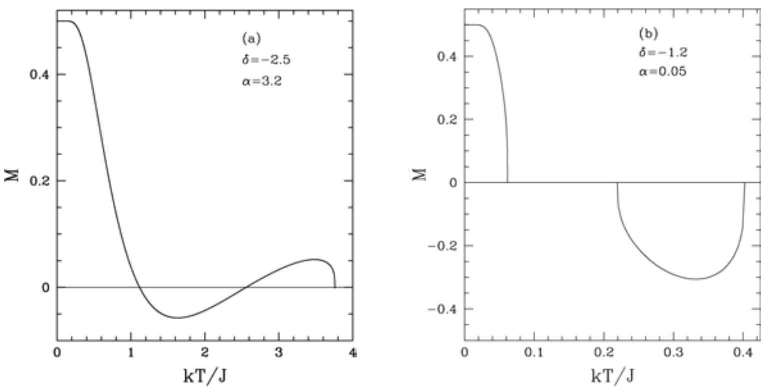

Fig. 4. (a) Total magnetization versus temperature for α = 3.2, δ = -2.5, showing two compensation points; (b) Total magnetization versus temperature for α = 0.05, δ = -1.2, showing three critical points.

Further details of this work, as well as an analysis of the $S = \frac{3}{2}$ case, are given in a forthcoming paper [9].

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