

An Ising ferrimagnetic model on a triangular lattice

This content has been downloaded from IOPscience. Please scroll down to see the full text.

1983 J. Phys. C: Solid State Phys. 16 3547

(<http://iopscience.iop.org/0022-3719/16/18/024>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 137.73.15.243

This content was downloaded on 02/03/2015 at 13:11

Please note that [terms and conditions apply](#).

An Ising ferrimagnetic model on a triangular lattice

D A Lavis and A G Quinn

Mathematics Department, Chelsea College, University of London, 552 King's Road, London SW10, UK

Received 24 December 1982

Abstract. We study a two-dimensional Ising model on a triangular lattice for which the lattice is divided into two sublattices, a honeycomb populated by ions of one species which interact with each other ferromagnetically and the remaining interstitial sites occupied by ions of different magnetic moment which interact with the first species antiferromagnetically. Exact results for the critical temperature and magnetisation on the zero-field axis are derived in special cases from the known results for the isotropic ferromagnetic Ising model. A real-space renormalisation method is used to obtain phase diagrams in the field–temperature plane together with the magnetisation and susceptibility on the zero-field axis. These latter exhibit the characteristic features of a ferrimagnetic system.

1. Introduction

Solids which have a net magnetic moment due to the incomplete cancellation of anti-ferromagnetically arranged spins are called ‘ferrimagnets’ of which a significant subgroup are the ferrites, these being ferromagnetic oxides with iron as their main metallic component. As was first shown by Néel (see e.g. Néel 1948, 1953) the magnetic ions in a ferrimagnet are situated at the sites of non-equivalent sublattices. In, for example, ferrites with spinel structure the lattice divides into two sublattices, one consisting of twice as many sites as the other. In ferrimagnets the exchange interactions are predominantly indirect. Differences in exchange energies between ions on different sublattices arise either because the lattice sites are occupied by ions of different types or because of the effects of different environments of non-magnetic atoms (see e.g. Wolf 1961, Martin 1967). One characteristic property of ferrimagnets is the shape of the inverse zero-field susceptibility curve above the critical temperature. Unlike the case of a ferromagnet this is normally concave towards the temperature axis and its high-temperature asymptote intercepts the axis at a point below the critical temperature. Another property of many ferrimagnets is the occurrence of a compensation temperature. This is a point on the zero-field axis below the critical temperature at which the magnetisation falls to zero owing to the cancellation of the sublattice magnetisations.

In this paper we consider a simple ferrimagnetic model on a triangular lattice of N sites. The lattice is divided into a honeycomb sublattice b of $2N/3$ sites and the triangular sublattice a consisting of the remaining $N/3$ sites of the original lattice. The sites of sublattices a and b are occupied by ions of magnetic moments ξ_a and ξ_b respectively. The nearest-neighbour exchange energies are $-J_{bb}$ and $-J_{ab}$ for b – b and a – b pairs respectively (there are of course no nearest-neighbour a – a pairs of sites). The interaction

within the b sublattice is ferromagnetic ($J_{bb} > 0$) and the interaction between sublattices is antiferromagnetic ($J_{ab} < 0$). We shall also consider the two limiting cases where either J_{bb} or J_{ab} , but not both, is zero. This is a model which has been considered by Bell (1974a, b) using high-temperature series expansions and, in some special cases, exact results. The purpose of this paper is to extend Bell's analysis of the exact results and to develop a real-space renormalisation-group (RSRG) method for the model.

2. Detailed model

Let an elementary nearest-neighbour triangle of the lattice consist of an a site with an ion in spin state S_a and two b sites b1 and b2 with ions in spin states S_{b1} and S_{b2} respectively. The possible values of S_a , S_{b1} and S_{b2} are +1 and -1 corresponding respectively to parallel and antiparallel alignment to the external magnetic field H . The Hamiltonian of the system is then

$$\mathcal{H} = \sum_{\Delta} \mathcal{H}_{\Delta} \tag{2.1a}$$

where

$$\mathcal{H}_{\Delta} = -[\tfrac{1}{2}(J_{ab}S_aS_{b1} + J_{ab}S_aS_{b2} + J_{bb}S_{b1}S_{b2}) + \tfrac{1}{6}H(\xi_aS_a + \xi_bS_{b1} + \xi_bS_{b2})] \tag{2.1b}$$

and the sum is over all the elementary triangles of the lattice.

The six possible ground states of the system are listed in table 1. The phases $F^{(+)}$ and $F^{(-)}$ are ferromagnetic, $F^{(+)}$ being more or less stable than $F^{(-)}$ at zero temperature according as the external magnetic field is greater or less than zero. When $H = 0$ the ferromagnetic phase is denoted by F. The degeneracy of this phase is 2 and it can be considered as the coexistence between large regions of the lattice in phases $F^{(+)}$ and $F^{(-)}$. The phases $AF^{(+)}$ and $AF^{(-)}$ are antiferromagnetic with respect to the spin alignment

Table 1. The ground states of the system.

Name	Configuration	Degeneracy ω_i	Hamiltonian $\mathcal{H}_{\Delta i}$ per Δ
(1) $F^{(+)}$		1	$-\tfrac{1}{2}(2J_{ab} + J_{bb})$ $-\tfrac{1}{6}H(2\xi_b + \xi_a)$
(2) $F^{(-)}$		1	$-\tfrac{1}{2}(2J_{ab} + J_{bb})$ $+\tfrac{1}{6}H(2\xi_b + \xi_a)$
(3) $AF^{(+)}$		2	$+\tfrac{1}{2}J_{bb} - \tfrac{1}{6}H\xi_a$
(4) $AF^{(-)}$		2	$+\tfrac{1}{2}J_{bb} + \tfrac{1}{6}H\xi_a$
(5) $FI^{(+)}$		1	$+\tfrac{1}{2}(2J_{ab} - J_{bb})$ $-\tfrac{1}{6}H(2\xi_b - \xi_a)$
(6) $FI^{(-)}$		1	$+\tfrac{1}{2}(2J_{ab} - J_{bb})$ $+\tfrac{1}{6}H(2\xi_b - \xi_a)$

the b sublattice, $AF^{(+)}$ being more or less stable than $AF^{(-)}$ at zero temperature according as the external field is greater or less than zero. When $H = 0$ the antiferromagnetic phase is denoted by AF. In this phase the directions of the spins on sublattice a are random. Except in the special case $J_{ab} = J_{bb}$ the degeneracy of this phase is $2^{(1+N/3)}$. When $J_{ab} = J_{bb}$ the distinction between sublattice sites disappears and we have the standard antiferromagnetic Ising model with ground-state degeneracy $(1.38135)^N$ (Wannier 1950). The phases $FI^{(+)}$ and $FI^{(-)}$ are ferrimagnetic. When $2\xi_b > \xi_a$ $FI^{(+)}$ is more or less stable than $FI^{(-)}$ at zero temperature according as the external field is greater or less than zero. If $2\xi_b < \xi_a$ the converse is the case. When $H = 0$ or $2\xi_b = \xi_a$ the ferrimagnetic phase is denoted by FI. This phase again has a degeneracy of 2 and consists of large regions of coexistence of $FI^{(+)}$ and $FI^{(-)}$. We define the parameters

$$\theta = J_{ab}/(J_{ab} - J_{bb}) \quad (2.2a)$$

and

$$r = \xi_a/\xi_b \quad (2.2b)$$

and the reduced temperature and field variables

$$\tilde{T} = kT/(J_{bb} - J_{ab}) \quad (2.3a)$$

and

$$\tilde{H} = \xi_b H/(J_{bb} - J_{ab}) \quad (2.3b)$$

respectively where k is Boltzmann's constant and T is the thermodynamic temperature. As indicated in § 1 we shall take $0 \leq \theta \leq 1$ for which the stable ground state at $\tilde{H} = 0$ is FI. In terms of the parameter r the stable ground states, with $\tilde{H} \neq 0$, can be obtained from table 1. They are, for $r < 2$, $F^{(-)}$, $FI^{(-)}$, $FI^{(+)}$, $F^{(+)}$ according as $\tilde{H} < -6\theta/r$, $-6\theta/r < \tilde{H} < 0$, $0 < \tilde{H} < 6\theta/r$, $6\theta/r < \tilde{H}$ and, for $r > 2$, $F^{(-)}$, $FI^{(+)}$, $FI^{(-)}$, $F^{(+)}$ according as $\tilde{H} < -3\theta$, $-3\theta < \tilde{H} < 0$, $0 < \tilde{H} < 3\theta$, $3\theta < \tilde{H}$. When $r = 2$ the phases $FI^{(+)}$ and $FI^{(-)}$ are degenerate. It may also be seen that at the points $\theta = 1.0$, $\tilde{H} = \pm 3.0$ the three phases $F^{(\pm)}$, $AF^{(\pm)}$, $FI^{(\mp)}$ are degenerate for all values of r . This does not affect the behaviour of the system for $r < 2$ since these points lie in the regions of stability of $FI^{(\pm)}$, but when $r > 2$ and $\theta = 1.0$ they correspond to the boundary between $FI^{(\mp)}$ and $F^{(\pm)}$ and lead (at least in our RSRG calculations, see § 5) to the phase diagrams for $\theta = 1.0$, differing from those for $1.0 > \theta > 0.0$.

Let $\xi_a m_a$ and $\xi_b m_b$ be the magnetisations per lattice site of the a and b sublattices respectively and let $\xi_b m$ be the magnetisation per lattice site of the whole lattice. Then

$$m = (2m_b + rm_a)/3. \quad (2.4)$$

It is clear that m_a , m_b and m are dimensionless magnetisations and for the sake of brevity we shall henceforth refer to them as magnetisations.

In this paper we shall be concerned with (a) the form of the phase boundaries in the $(\tilde{T}, \tilde{H})$ plane and (b) the behaviour of the magnetisation m and the isothermal susceptibility χ_T for $\tilde{H} = 0$, for different values of θ and r . The susceptibility is given by

$$\chi_T = \chi_0 (\partial m / \partial \tilde{H})_{\tilde{T}} \quad (2.5a)$$

where

$$\chi_0 = \xi_b^2 / [\mu_0 V_0 (J_{bb} - J_{ab})]. \quad (2.5b)$$

μ_0 is the permeability of free space and V_0 is the area per lattice site.

Before investigating these using a RSRG method we shall, in § 3, summarise the exact results that can be derived for the model from the known results for the isotropic ferromagnetic Ising (IFI) model.

3. Exact results

3.1. $\theta = 0.0$ ($J_{ab} = 0$, $J_{bb} > 0$)

This case differs from the standard ferromagnetic honeycomb model only in that there are uncoupled ions on the a sites. The effect of these is to augment the magnetisation in non-zero field with a paramagnetic contribution. The Curie temperature can be calculated from that of the IFI model using the star-triangle transformation (see e.g. Syozi 1972). The transformation yields

$$\cosh[2J_{bb}/(kT)] = \frac{1}{2}\{1 + \exp[4J_F/(kT)]\} \quad (3.1)$$

where $J_F > 0$ is the interaction energy of the IFI model. With the Curie temperature of that model given by $\exp[4J_F/(kT_c)] = 3$ we have $\tilde{T}_c = 1.519$ for the Curie temperature in this case.

3.2. $\theta = 0.5$ ($J_{bb} = -J_{ab} > 0$)

This and the next case were considered by Bell (1974a, b). When $\tilde{H} = 0$ the magnetisations per lattice site are given by

$$m_a = -rm_F \quad (3.2a)$$

$$m_b = m_F \quad (3.2b)$$

for the a and b sublattices respectively, where m_F is the magnetisation per lattice site of an IFI model with magnetic moment per ion ξ_b and ferromagnetic interaction J_{bb} . The overall magnetisation per site is

$$m = m_F(2 - r)/3. \quad (3.3)$$

The formula for m_F was derived by Wannier (1950) and Houtappel (1950). It can be expressed in the form

$$m_F = \pm \left(\frac{(1+u)^3(1-3u)}{(1-u)^3(1+3u)} \right)^{1/8} \quad (3.4)$$

where $u = \exp[-4J_{bb}/(kT)]$. Unless $r = 2$ the critical temperature is that of the IFI model. If we consider the limit $\tilde{H} \rightarrow 0+$ then the transition is to a phase for which $m > 0$. If $r < 2$ we choose the positive sign in (3.4) and the transition is to $\text{FI}^{(+)}$; if $r > 2$ we choose the negative sign in (3.4) and the transition is to $\text{FI}^{(-)}$. In both cases the critical temperature is given by $3u_c = 1$, $\tilde{T}_c = 1.820$ and below the critical temperature there is a first-order transition between $\text{FI}^{(+)}$ and $\text{FI}^{(-)}$ as $\tilde{H}$ passes through zero. Bell (1974a) used an argument of Fisher (1959) to show that, unless $r = 2$, the critical index γ is equal to that of the IFI model. When $\tilde{H} \neq 0$ the simple mapping between this and the IFI model no longer holds.

3.3. $\theta = 1.0$ ($J_{bb} = 0$, $J_{ab} < 0$)

In this case the model reduces to a triangular lattice of ions on the a sites which interact indirectly via the b sites situated at the centres of each triangle. The model can be related to an IFI model on the a sites by means of a modified star-triangle transformation in which the partition function is summed over the spin states on the b sites. It is not difficult to show that when $\tilde{H} = 0$ there is a one-to-one mapping between $J_{ab}/(kT)$ and $J_F/(kT)$. This is in contrast to the rather similar Kagomé lattice model of Bell (1974b). There a dedecoration transformation yielded a mapping which was not one-to-one. The zero-field axis of the IFI model mapped both into the zero-field axis of the ferrimagnetic model and into a line in the phase plane where the field was non-zero. For the present model the transformation gives

$$\cosh[2J_{ab}/(kT)] = \frac{1}{2}\{1 + \exp[2J_F/(kT)]\} \quad (3.5)$$

and we have the critical temperature $\tilde{T}_c = 2.405$.

For non-zero field the situation is rather more complicated. The presence of odd-degree terms in the Hamiltonian leads to the generation of a three-spin coupling in the IFI model as well as the usual two-spin and single-spin terms. In order to obtain a self-consistent three-parameter mapping between models we must introduce a three-spin coupling between the b-site ions and pairs of neighbouring a-site ions in the ferrimagnetic model. Setting this interaction to zero means that we then have a mapping from the original model on to a surface $\mathcal{S}$ in the three-dimensional phase space Λ of the IFI model with three-spin coupling. If the critical surfaces in Λ were known then the critical curves of the ferrimagnetic model would be given by their intersections with $\mathcal{S}$. However the only exact information available is on the pure two-spin axis for which there is a first-order transition below the Curie temperature and on the pure three-spin axis where there is a first-order transition below the Baxter-Wu temperature (Baxter and Wu 1973, 1974). Parts of the rest of the space have been investigated using renormalisation-group methods (Imbro and Hemmer 1976, den Nijs *et al* 1976, Schick *et al* 1977) but the results are by no means decisive.

Since the work of Bell (1974a, b) was published Baxter (1975) has obtained a formula for the three-spin correlation function m_{F3} of the IFI model in zero field. This allows us to obtain the sublattice magnetisations for our model. If the moments of the ions of the IFI model are ζ_b we have

$$m_a = r m_F \quad (3.6a)$$

$$m_b = \left(\frac{c-1}{2c-1}\right) \left(\frac{c-1}{c+1}\right)^{1/2} \left[\frac{3m_F c}{(c-1)} - m_{F3}\right] \quad (3.6b)$$

where $c = \cosh[2J_{ab}/(kT)]$, m_F is given by (3.4) and

$$m_{F3} = m_F \left[3 \left(\frac{1+u}{1-u} \right) - 2 \left(\frac{1+3u}{(1-u)^3} \right)^{1/2} \right] \quad (3.7)$$

(see Baxter 1975). The variable $u = \exp[-4J_F/(kT)]$ which appears in (3.4) and (3.7) is, from (3.5), now given by $u = (2c-1)^{-2}$. From (2.4), (3.4), (3.6) and (3.7) we are able to obtain an expression for the magnetisation m per lattice site. If we consider the side of the temperature axis $\tilde{H} = 0+$ then $m > 0$ and at zero temperature since $|m_a| = |m_b| = 1$, $m_a = -m_b$, we see that we must choose $m_F < 0$, > 0 according as $r < 2$, > 2 . The phase at zero temperature is $\text{FI}^{(+)}$, $\text{FI}^{(-)}$ according as $r < 2$, > 2 . Retaining the

choice of sign in (3.4) the formula for m is

$$m = \pm \frac{1}{3} \left(\frac{(2c^2 - 2c + 1)^3 (2c^2 - 2c - 1)}{16c^3 (c - 1)^3 (c^2 - c + 1)} \right)^{1/8} \times \left\{ r + \frac{(c^2 - 1)^{1/2}}{c(c + 1)} \left[3 + (2c - 1) \left(\frac{c^3 + 1}{c^3 - c} \right)^{1/2} \right] \right\}. \quad (3.8)$$

In the neighbourhood of the critical temperature this has the asymptotic form

$$m \sim \mp (16/\tilde{T}_c^2) (\tilde{T}_c - T)^{1/8} [(r^* - r) + (36/\tilde{T}_c^2) (\tilde{T}_c - \tilde{T})] \quad (3.9)$$

where

$$r^* = 4(\sqrt{3}/2)^{1/2} (2\sqrt{3} - 3) = 1.7276. \quad (3.10)$$

The critical exponent β has the same value $1/8$ as for the IFI model unless $r = r^*$ when it has the value $9/8$.

For $r < r^*$ the choice in (3.9) is the lower sign corresponding to $m_F < 0$ ($m_a < 0$, $m_b > 0$) and the phase transition is to $\text{FI}^{(+)}$, this phase persisting to zero temperature. For $r > 2 > r^*$ the choice in (3.9) is the upper sign with $m_F > 0$ ($m_a > 0$, $m_b < 0$) and the phase transition is to $\text{FI}^{(-)}$ with this phase persisting to zero temperature. The interesting range is $r^* < r < 2$. Here the transition is to $\text{FI}^{(-)}$ ($m_F > 0$) but the zero-temperature phase is $\text{FI}^{(+)}$. A curve representing the transition between these phases must leave the zero-field axis at the compensation temperature $\tilde{T}^*$ where $m = 0$. Since $m_a \neq 0$ (and $m_b \neq 0$) at $\tilde{T} = \tilde{T}^*$ these variables must change discontinuously corresponding to a first-order phase transition. Curves of magnetisation against temperature derived from (3.8) with the appropriate choice of sign are shown in figure 1.

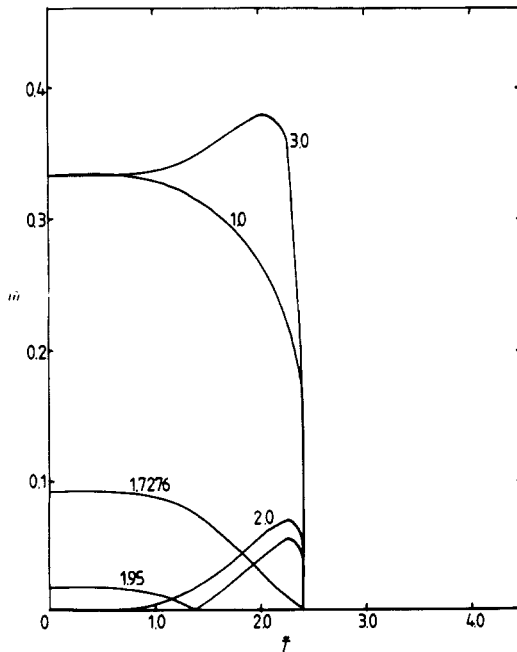


Figure 1. Curves of the magnetisation per lattice site as a function of temperature derived from the exact formula (3.8), for various values of r when $\theta = 0$ ($J_{bb} = 0$).

In general $r^* = r^*(\theta)$ is defined to be the value of r as a function of θ for which the transition to the ferrimagnetic phase for $\tilde{H} = 0+$ or $0-$ changes between $\text{FI}^{(-)}$ and $\text{FI}^{(+)}$. We know on the basis of the exact results given above that $r^*(0.5) = 2.0$ and $r^*(1.0) = 1.7276$. In general we define the compensation temperature $\tilde{T}^* = \tilde{T}^*(r, \theta)$ as the point at which a line of first-order $\text{FI}^{(+)}\text{--FI}^{(-)}$ transitions leaves the zero-field axis. We know that $T^*(r, 1.0)$ exists when $r^* < r < 2$ and from figure 1, we see that $\tilde{T}^* \rightarrow \tilde{T}_c$ as $r \rightarrow r^*$ and $\tilde{T}^* \rightarrow 0$ as $r \rightarrow 2$. In § 4 we shall investigate r^* and $\tilde{T}^*$ more generally using an approximate RSRG procedure.

4. Renormalisation method

We use the block-spin transformation employed by Schick *et al* (1977). In the most general form of this method the triangular lattice is divided into three equivalent triangular sublattices A, B and C with three different nearest-neighbour interactions between pairs of sites on different sublattices and three different magnetic moments for the ions on the three sublattices. A three-spin interaction must also be included since it is generated by the transformation and, taking into account the trivial interaction, we have a transformation with eight variables corresponding to the eight ground states of the general model. An initial cluster of nine sites is chosen with three sites belonging to each sublattice and periodic boundary conditions are imposed. Application of the RSRG transformation reduces the nine-site cluster to a cluster of three sites, one belonging to each sublattice. This corresponds to an increase in length scale by a factor $\sqrt{3}$. The spin state on the renormalised α' site ($\alpha = \text{A, B, C}$) is determined by the spin states on the three α -sites in the nine-site cluster using the 'majority-rule' weight function.

The same cluster method has been used by Schick and Griffiths (1977) for the three-state Potts model, by Young and Lavis (1979) and Southern and Lavis (1980) for models with directional bonding, by Southern and Lavis (1979) for a model of adsorbed molecules and by Lavis *et al* (1982) for the spin-1 Ising model applied to monolayers at air/water on oil/water interfaces. Reference could be made to these papers for a more detailed account of the method.

The renormalisation transformation represents a semi-group of transformations in the eight-dimensional space of dimensionless couplings. A four-dimensional invariant subspace of the transformation is that of the IFI model investigated in detail by Schick *et al* (1977). Our present model, in which sublattice A is identified with a and B and C together with b corresponds to a six-dimensional invariant subspace. Let $\mathcal{H}_{\Delta i}$, $i = 1, \dots, 6$ be the ground-state Hamiltonians listed in table 1 augmented by a three-spin term $-QS_a S_{b1} S_{b2}$. If the renormalisation procedure is now applied to the six variables $x_i = \exp(-\mathcal{H}_{\Delta i}/kT)$ the transformation equations for x_1, x_3, x_5 are

$$x_0'^6 x_1'^6 = x_1^{18} + 3x_1^{12} x_3^6 + 6x_1^{12} x_3^6 + 18x_1^8 x_3^4 x_4^2 x_5^4 + 9x_1^8 x_3^8 x_6^2 \\ + 9x_1^6 x_3^4 x_4^2 x_5^2 x_6^2 + 18x_1^5 x_2 x_3^6 x_4^2 x_5^3 x_6 \quad (4.1a)$$

$$x_0'^6 x_3'^6 = x_3^{18} + 3x_3^{12} x_4^6 + 3x_3^{12} x_6^6 + 9x_3^8 x_3^8 x_4^4 x_6^4 + 3x_3^6 x_3^{12} + 9x_1^4 x_3^8 x_4^4 x_5^2 \\ + 9x_1^4 x_3^{10} x_4^6 + 9x_1^2 x_2^2 x_3^8 x_4^2 x_5^2 x_6^2 + 18x_1^3 x_2 x_3^6 x_4^4 x_5 x_6^3 \quad (4.1b)$$

$$x_0'^6 x_5'^6 = x_5^{18} + 3x_1^6 x_5^{12} + 6x_1^6 x_5^{12} + 18x_1^4 x_3^2 x_4^4 x_5^8 + 9x_2^2 x_4^8 x_5^8 \\ + 9x_1^2 x_2^2 x_3^4 x_4^6 x_5^6 + 18x_1^3 x_2 x_3^2 x_4^6 x_5^5 x_6. \quad (4.1c)$$

Those for x_2 , x_4 and x_6 are obtained by the interchanges $x_1 \leftrightarrow x_2$, $x_3 \leftrightarrow x_4$, $x_5 \leftrightarrow x_6$. The variable x'_0 arises from the renormalisation of the trivial interaction referred to above. It is determined by the condition that

$$\sum_{i=1}^6 \omega_i \overline{\mathcal{H}}_{\Delta i} = 0 \quad (4.2a)$$

(see table 1) or equivalently

$$\prod_{i=1}^6 x_i^{\omega_i} = 1 \quad (4.2b)$$

at each stage of the iteration process, when the ω_i are the degeneracies given in table 1. The variable x_0 is important for calculating the free energy and its derivatives (see § 6) but plays no part in determining the phase diagram which can be obtained from a consideration of the trajectories in the space $\{x_1, x_2, \dots, x_6\}$. A trajectory which begins at a point which is not critical will iterate to a sink which characterises the phase. These regions are separated by the critical regions which form domains of attraction for the critical fixed points. An interesting computational problem arises in implementing this procedure; that is that most of the sinks and some of the critical fixed points have locations in the space $\{x_i\}$ which, while satisfying (4.2b), have some x_i zero and some infinite. Our method of overcoming this difficulty is as follows. Equations (4.1) can be represented in the form

$$x_0^{(k+1)6} x_i^{(k+1)6} = Z_i(x_i^{(k)}) \quad k = 0, 1, 2, \dots \quad (4.3)$$

where Z_i , $i = 1, \dots, 6$ are homogeneous polynomials of degree 18, k is an index for a succession of points along a trajectory, and condition (4.2b) is satisfied for the coordinates $\{x_i^{(k)}\}$ $k = 0, 1, 2, \dots$. Now suppose equations (4.3) are replaced by

$$z_0^{(k+1)6} z_i^{(k+1)6} = Z_i(z_i^{(k)}) \quad k = 0, 1, 2, \dots \quad (4.4)$$

where $z_i^{(0)} = x_i^{(0)}$, $i = 1, \dots, 6$, but instead of (4.2b) we now impose the condition that the largest $z_i^{(k)}$ for $k = 1, 2, \dots$ is unity. This means that

$$z_0^{(k+1)} = [Z_{\max}(z_i^{(k)})]^{1/6}. \quad (4.5)$$

The variables z_i remain finite along a trajectory and

$$x_i^{(k)} = z_i^{(k)} / \alpha^{(k)} \quad i = 1, \dots, 6 \quad (4.6a)$$

$$x_0^{(k)} = \alpha^{(k)} z_0^{(k)} / \alpha^{(k-1)3} \quad (4.6b)$$

where

$$\alpha^{(k)} = \left(\prod_{i=1}^6 z_i^{(k)\omega_i} \right)^{1/6}. \quad (4.7)$$

The fixed points discussed in § 5 are described in table 2 in terms of their coordinates in the space $\{z_i\}$. Once these fixed points have been located the recurrence relations can be linearised about them and the eigenvalues λ_i of the linear equations can be calculated. The critical exponents y_i are related to the eigenvalues by $\lambda_i = b^{y_i}$ where b is the scale factor which is $\sqrt{3}$ in the present calculation. For a sink all the critical exponents are negative (irrelevant). A fixed point controlling a critical surface separating two phases

Table 2. Fixed points.

Name	Coordinates						Relevant exponents		
	z_1	z_2	z_3	z_4	z_5	z_6	Even subspace		
P	1.0	1.0	1.0	1.0	1.0	1.0	0.6381 0.6179 0.7381	0.4799	0.7381 0.7381
FIS	0.0	0.0	0.0	0.0	1.0	1.0			2.0
C	0.6907	0.6907	0.6907	0.6907	1.0	1.0			1.4544 0.5946
R	1.0	1.0	0.5970	0.5970	1.0	1.0			1.7418 0.7381
O	1.0	1.0	0.0	0.0	1.0	1.0			2.0 0.7381
D	1.0	0.0	0.0	0.0	1.0	0.0	0.7381		
X	0.8910	0.0	0.0	0.0	0.8910	1.0	2.0	0.7381	
L	1.0	0.0	1.0	0.0	0.0	1.0	0.7381		
K	1.0	0.0	0.0	0.0	0.0	1.0	2.0		
M	1.0	0.0	0.5970	0.0	0.0	1.0	1.7418	0.6179	

will have one positive (relevant) exponent. An exponent $y_i = d = 2$ is a necessary condition for a first-order phase transition (Nienhuis and Nauenberg 1975) and an exponent $1 = d/2 < y_i < d = 2$ is a necessary condition for divergence of the susceptibility. In order to determine whether a discontinuity in magnetisation or a singularity in the susceptibility actually occurs it is necessary to determine these thermodynamic functions using the techniques described in § 6.

5. Phase diagrams

If $\tilde{H} = 0$ ($Q = 0$) the Hamiltonian contains only even-degree terms. This is a three-dimensional invariant subspace of the renormalisation transformation (4.1), with $x_1 = x_2$, $x_3 = x_4$, $x_5 = x_6$, which can be represented as the $(\tilde{T}, \theta)$ plane. For $0.0 < \theta \leq 1.0$ the group under which the Hamiltonian is invariant is $\mathcal{S}_2$, the group of two elements one of which is the inversion of all spins on the lattice. For $\theta = 0$ the symmetry group of the Hamiltonian is the group of $2^{(N/3+1)}$ elements $\mathcal{S}_2^{(b)} \otimes \mathcal{S}_2^{(a_1)} \otimes \dots \otimes \mathcal{S}_2^{(a_{N/3})}$ where $\mathcal{S}_2^{(b)}$ is the group $\mathcal{S}_2$ applied to all the sites of sublattice b and $\mathcal{S}_2^{(a_i)}$ is the group $\mathcal{S}_2$ applied to the i th site of sublattice a for $i = 1, 2, \dots, N/3$. This leads to the expectation that the transforms to spin ordering for $0 < \theta \leq 1$ will be controlled by one fixed point and that for $\theta = 0$ by another. Since $\theta = 0.5$ ($J_{bb} = -J_{ab} > 0$) can be obtained from the IFI model by changing the sign of J_{ab} and inverting the spins on the a sublattice it is an invariant line in the $(\tilde{T}, \theta)$ plane. We therefore expect the fixed point which controls the ordering transition for $0 < \theta \leq 1$ to be on this line and to have an even exponent which places it in the universality class of the IFM. These general expectations are confirmed by our numerical calculations using the renormalisation transformation (4.1) (see figure 2). At the high temperatures trajectories iterate to the paramagnetic fixed point P and at low temperatures for $\theta \neq 0$ trajectories iterate to the fixed point FIS. Neither of these has any relevant even exponents (see table 2) and they are therefore sinks relative to the plane $\tilde{H} = 0$. The relevant odd exponent 2.0 of FIS is indicative of the fact that the plane $\tilde{H} = 0$ for $\tilde{T} < \tilde{T}_c$ is a surface of first-order transitions between $\text{FI}^{(+)}$ and $\text{FI}^{(-)}$. These two regions are separated by a critical curve controlled by the fixed point C which lies at $\theta = 0.5$, $\tilde{T} = 2.703$. This temperature is the same as the Curie temperature of the IFM obtained by Schick *et al* (1977) as is also the even exponent 0.6381. For $\theta = 0$ the transition is from the paramagnetic phase to a line of coexistence of F and FI. The fixed

point controlling this transition is R which lies at $\theta = 0.0$, $\tilde{T} = 1.9385$. This fixed point has two relevant even exponents 0.6179 and 0.4799, the former being the thermal exponent and the latter the exponent which drives trajectories along the critical curve to the fixed point C. Trajectories on the line $\theta = 0$ for subcritical temperatures are driven towards the fixed point O at $\tilde{T} = 0$. This has one relevant even exponent 0.7381 corresponding to a continuous transition between F and FI as θ passes through zero.

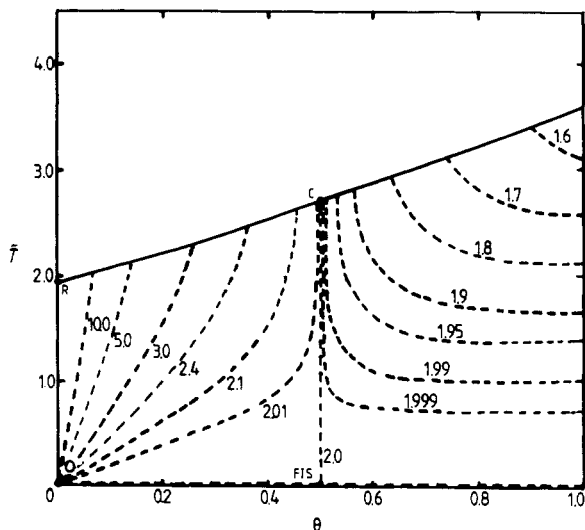


Figure 2. Behaviour of the system in the $(\tilde{T}, \theta)$ plane derived from the RSRG calculations. The full curve is the critical temperature on which the trajectory flow is towards the fixed point C. The broken curves parametrised by r give the values of the compensation temperature $\tilde{T}^*(r, \theta)$.

For $\tilde{H} \neq 0$ the exact calculations of § 4 lead us to expect that there exists an $r^*(\theta)$ such that for r lying between r^* and 2 there is a temperature $\tilde{T}^*(r, \theta)$ at which a first-order $\text{FI}^{(+)}\text{--FI}^{(-)}$ transition leaves the $\tilde{H} = 0$ axis. To determine r^* as a function of θ we adopted the following strategy. For a fixed value of r we obtained the temperature of the $\text{FI}^{(+)}\text{--FI}^{(-)}$ transition for small $\tilde{H}$ at varying values of θ . This gives us a family of curves in the $(\tilde{T}, \theta)$ plane (see figure 2) parametrised by r . The point at which a particular curve joins the critical curve then gives us the value of θ for which this r is r^* . From this a curve of r^* as a function of θ is obtained (see figure 3). We can distinguish four regions A, B, C and D of the (r, θ) plane within which the phase diagrams are qualitatively similar. In region A, where for $0 < \theta \leq 0.5$, $r < 2$ and for $0.5 < \theta \leq 1$, $r < r^*$, the ground state for $0 < \tilde{H} < 6\theta/r$ is $\text{FI}^{(+)}$. A typical diagram of this type, with $\theta = 1.0$, $r = 1.0$, is given in figure 4(a). Below the critical temperature $\tilde{T}_c(\theta)$ on the zero-field axis there is a first-order transition between $\text{FI}^{(+)}$ and $\text{FI}^{(-)}$ controlled by the fixed point FIS. The transition between $\text{FI}^{(+)}$ and $\text{F}^{(+)}$ is continuous. It follows the zero-field axis to a temperature $\tilde{T}_0(r, \theta)$ and then leaves the axis eventually terminating at $\tilde{T} = 0.0$, $\tilde{H} = 6\theta/r$. The fixed point controlling this transition is D. Since the one relevant exponent of this fixed point is less than unity the transition is not second-order, there being no singularity in the susceptibility. Its principal characteristic is that m_a passes continuously through zero (see § 6). As r approaches r^* from below, $\tilde{T}_0$ approaches $\tilde{T}_c$ from above. As we cross the

curve $r = r^*$ in figure 3 into *region B* a region of stability of $\text{FI}^{(-)}$ makes its appearance. Figure 4(b) with $\theta = 1.0$, $r = 1.9$, is a typical diagram of this type. The $\text{FI}^{(+)}\text{--F}^{(+)}$ transition is continuous and still controlled by the fixed point D. This curve coalesces with the line of first-order $\text{FI}^{(+)}\text{--FI}^{(-)}$ transitions which leaves the zero-field axis at the compensation temperature $\tilde{T}^*$, and a curve of continuous $\text{FI}^{(-)}\text{--F}^{(+)}$ transitions at an end-point controlled by the fixed point C. The line of first-order transitions is controlled by FIS. The

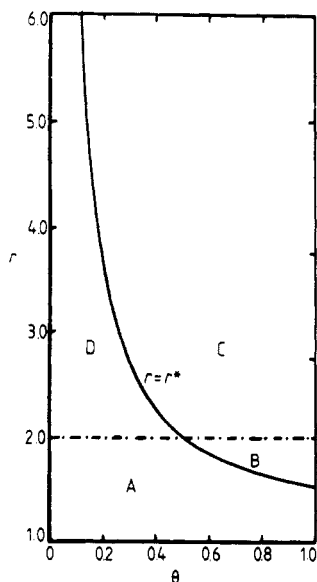
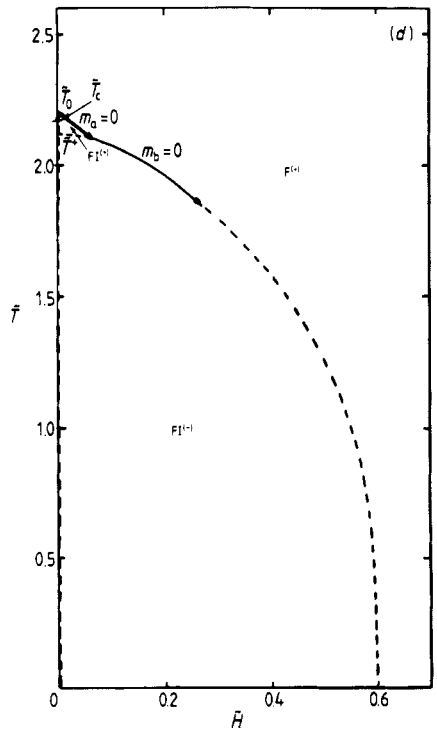
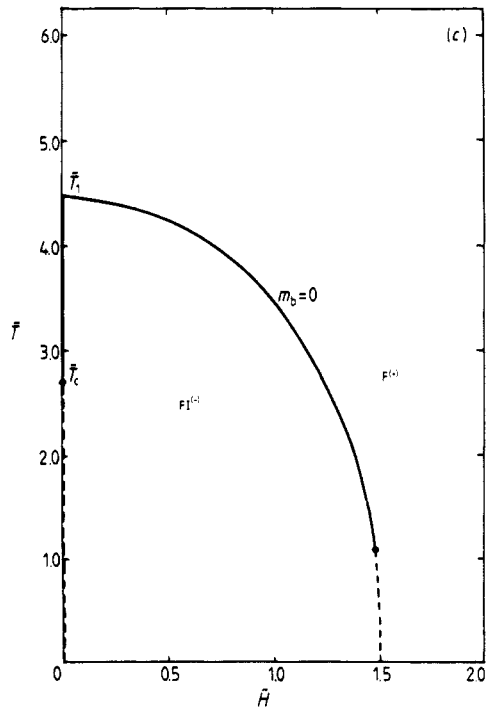
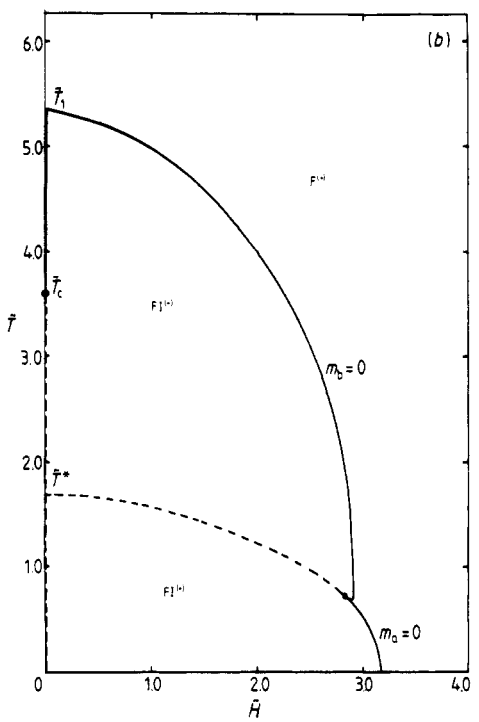
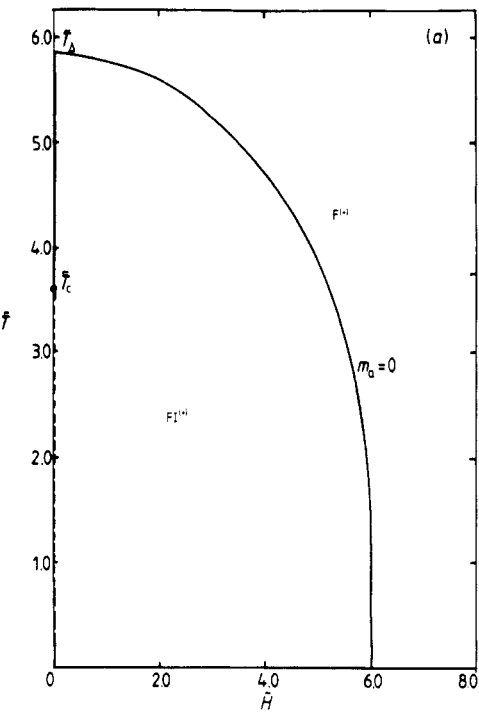


Figure 3. The regions A, B, C and D in the (r, θ) plane which exhibit qualitatively different phase diagrams. The curve $r = r^*$ is derived from figure 2 as described in the text.

continuous $\text{FI}^{(-)}\text{--F}^{(+)}$ transition, like the $\text{FI}^{(+)}\text{--F}^{(+)}$ transition in figure 4(a), follows the zero-field axis above the critical temperature until, in this case, it attains a temperature $\tilde{T}_1(r, \theta)$ when it leaves the axis. The fixed point controlling this transition is L. Its one relevant exponent is the same as that of D. The transition is weaker than second-order and is marked by m_b passing through zero. As r tends towards 2 from region B, $\tilde{T}^*$ tends to zero and when we pass into *region C* where the stable ground state for $0 < \tilde{H} < 3\theta$ is $\text{FI}^{(-)}$. As was indicated by our discussion in § 2 a difference occurs in this region according to whether $\theta = 1.0$ or $1.0 > \theta > 0.0$. In the former case the phase bounding between $\text{FI}^{(-)}$ and $\text{F}^{(+)}$ meets the zero-temperature axis at a point where these phases are degenerate with $\text{AF}^{(+)}$. The consequence of this is that the fixed point L with equal weights in phases 1, 3 and 6 controls the $\text{FI}^{(-)}\text{--F}^{(+)}$ transition for all temperatures. The phase diagram would have the same rather uninteresting appearance as figure 4(a) with a weak continuous transition, which in this case is marked by m_b passing through zero. When $\theta \neq 1.0$ the behaviour changes. A typical diagram of this type, with $\theta = 0.5$, $r = 3.0$, is given in figure 4(c). The $\text{FI}^{(-)}\text{--F}^{(+)}$ transition is first-order at low temperatures and is controlled by the fixed point K. At high temperatures it is still controlled by L. These two parts of the curve join at a point controlled by fixed point M. In *region D* two types of phase behaviour are exhibited. As the region is entered from region C (by, for example, reducing r through r^* at constant θ) the phase $\text{FI}^{(+)}$ appears in the neighbourhood of the



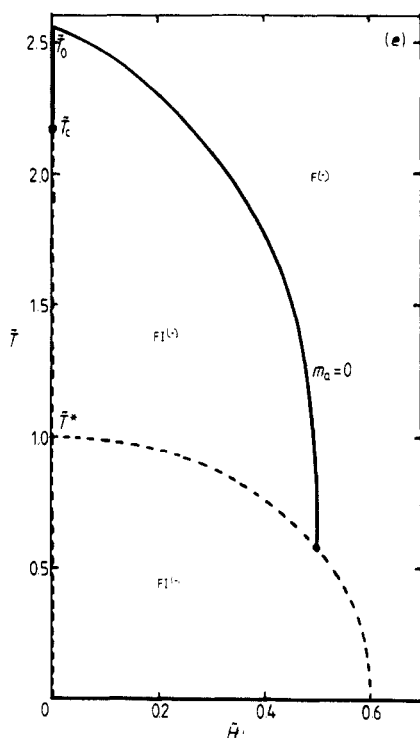


Figure 4. Phase diagrams in the $(\tilde{T}, \tilde{H})$ plane for (a) $\theta = 1.0$, $r = 1.0$; (b) $\theta = 1.0$, $r = 1.9$; (c) $\theta = 0.5$, $r = 3.0$; (d) $\theta = 0.2$, $r = 3.575$; (e) $\theta = 0.2$, $r = 2.4$. Broken curves represent first-order phase transitions, full curves are weak continuous transitions across which one or both of the sublattice magnetisations pass through zero.

critical point. A typical phase diagram of this type is given in figure 4(d), where $\theta = 0.2$, $r = 3.575$. The first-order $\text{FI}^{(-)}\text{--FI}^{(-)}$ transition is again controlled by FIS with the end-point controlled by C. The continuous $\text{FI}^{(+)}\text{--F}^{(+)}$ transition is controlled by D. As r is further reduced the continuous $\text{FI}^{(+)}\text{--F}^{(+)}$ transition contracts until the end-points of the two first-order transitions coalesce and their meeting point, which is also the end of the continuous $\text{FI}^{(+)}\text{--F}^{(+)}$ transition, is controlled by fixed point x. A typical diagram of this type is given in figure 4(e) where $\theta = 0.2$, $r = 2.4$. As r is further reduced to 2 the $\text{FI}^{(+)}$ phase contracts towards the zero-temperature axis and we return to region A.

It is not difficult to understand why the low-temperature $\text{FI}^{(+)}\text{--F}^{(+)}$ transition is continuous while the $\text{FI}^{(-)}\text{--F}^{(+)}$ transition, except when $\theta = 1.0$, is first-order. In the first case the transition involves reversing the spins on the a sublattice. These are non-interacting spins. The $\text{FI}^{(-)}\text{--F}^{(+)}$ transition involves reversing the network of interacting spins on the b sublattice. When $\theta = 1.0$ ($J_{bb} = 0$) the spins on the b sublattice are non-interacting and in this case a continuous transition is not unexpected.

6. Thermodynamic functions

In § 5 we have referred to the behaviour of the magnetisation on the critical curves in the $(\tilde{T}, \tilde{H})$ plane. In this section we describe the method of obtaining this magnetisation and the susceptibility. The partition function Z associated with the initial cluster of nine

sites is given by

$$Z = \sum_{i=1}^6 \omega_i Z_i(x_j) \quad (6.1)$$

where Z_i are the polynomial functions appearing in (4.3) and (4.4). After the RSRG transformation has been applied the partition function Z' associated with the remaining cluster of three sites is

$$Z' = \sum_{i=1}^6 \omega_i (x'_i)^6. \quad (6.2)$$

Using (4.3) we find that the free energies per site are related by

$$f = \frac{1}{3}f' - \frac{2}{3} \ln x'_0 \quad (6.3)$$

where $f = -\frac{1}{3} \ln Z$ and $f' = -\frac{1}{3} \ln Z'$. Substituting from (4.6b) and iterating (6.3) we have

$$f = -2 \sum_{k=1}^{\infty} \frac{1}{3^k} \ln z_0^{(k)}. \quad (6.4)$$

In practice this infinite series converges very quickly and the free energy at the initial point $x_i^{(0)} = z_i^{(0)}$ can be obtained after only a few iterations. The sublattice magnetisations at the initial point on the trajectory are now given by

$$m_\tau = -\partial f / \partial \zeta_\tau \quad \tau = a, b \quad (6.5)$$

where $\zeta_\tau = \xi_\tau H / kT$, and the overall magnetisation and susceptibility are given by (2.4) and (2.5). Curves of magnetisation and inverse susceptibility for typical cases are given in figures 5 and 6 respectively. Figure 5 should be compared with the exact results for the same case shown in figure 1. The values of the critical temperature and r^* differ in these two calculations but the curves are qualitatively similar. The curves for magnetisation remain of the same general form for $0.5 < \theta \leq 1$. When $\theta \leq 0.5$ there are of course no curves on which there is a compensation temperature at which $m = 0$. The curves of inverse susceptibility shown in figure 6 all have a zero at the critical temperature except when $r = r^*$ ($= 1.508$ in this case). The value of the critical exponent γ calculated from the exponents of fixed point c is 1.424. The absence of a singularity in the susceptibility at $r = r^*$ is presumably because this value of r is that for which the amplitude of the singular term is zero in the same way as the amplitude of the leading term in the magnetisation in (3.9) is zero for this value. Given that this model for all $0 < \theta \leq 1$ is in fact in the same universality class as $\theta = 0.5$ then, as indicated above, except when $r = 2$, the exact value of γ is that of the IFI model, namely 1.75. Within the context of the present method the fixed point controlling the spin-ordering transition on the zero-field axis is unaffected by changes in the value of r . We are therefore unable to obtain a different critical exponent γ in the case $r = 2$.

7. Conclusions

We have investigated a simple two-dimensional model which, like the ferrites with spinel structure, consists of two sublattices of spins with an antiferromagnetic interaction between sublattices. Exact results for the isotropic ferromagnetic Ising model allow us to deduce the existence of a compensation temperature within a certain range of the ratio of magnetic moments. From this we may infer the presence of a first-order phase

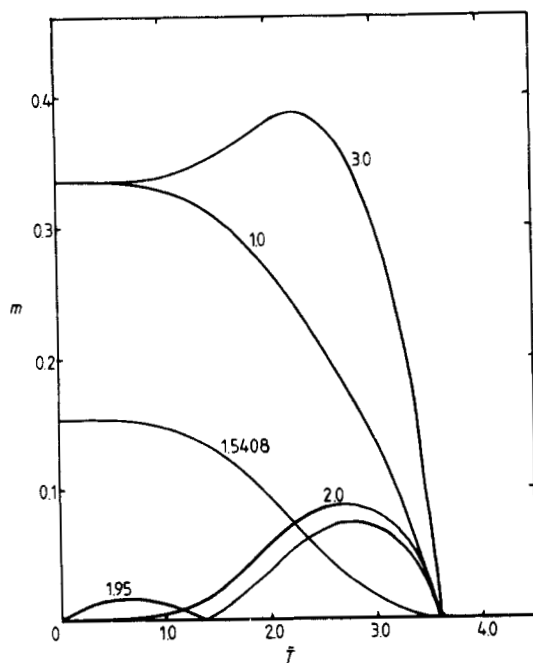


Figure 5. Curves of magnetisation per lattice site as a function of temperature, derived from the RSRG calculations for various values of r when $\theta = 0$ ($J_{bb} = 0$).

transition leaving the zero-field axis at this point. The RSRG method which we have used is of course an approximation but its results are in qualitative agreement with the exact results.

Using a different but similar model based on a Kagomé lattice Bell (1974b) obtained

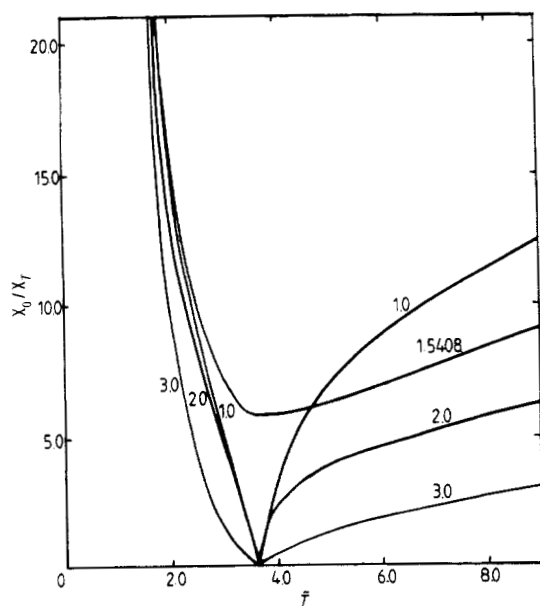


Figure 6. Curves of reduced inverse isothermal susceptibility as a function of temperature derived from the RSRG calculations for various values of r when $\theta = 0$ ($J_{bb} = 0$).

exact results corresponding to cases of our model with (i) $J_{bb} = -J_{ab} > 0$ and (ii) $J_{bb} = 0, J_{ab} < 0$. He restricted himself to the range $r \leq N_b/N_a$, where N_a and N_b are respectively the number of sites on the a and b sublattices, and obtained phase diagrams in case (ii) very similar to our own. He posed the question as to whether case (i) or case (ii) represents the typical behaviour for different values of θ and suggested the latter on the basis of mean-field calculations. The same question can equally well be asked with respect to our model and an answer is clearly given by our RSRG calculations, although of course it may be modified by subsequent exact results. For $r < N_b/N_a = 2$ the case $\theta = 1.0$ is typical in the range $0.5 < \theta \leq 1$ where we are in region A or B (see figure 3). When $r > 2$, $\theta = 1.0$ is a special case for which no first-order $F^{(+)}-F^{(-)}$ transition occurs. The case $\theta = 0.5$ is a special case in the sense that with respect to the whole range of r it is unique. It is however typical of the region C for $r > 2$ and of region A for $r < 2$. The types of behaviour exhibited in figures 4(d) and 4(e) for region D do not occur for any values of r for either of the two cases $\theta = 0.5$ or $\theta = 1.0$.

It is well known that RSRG methods of the type used here, where relatively few sites are divided into sublattices, give rather poor agreement with exact results for ferromagnetic critical temperatures and exponents. This deficiency of the method carries over to our investigation of ferrimagnets. We have nevertheless been able to predict the existence of compensation temperatures and obtain curves for the inverse susceptibility above the critical temperature which are, as in real ferrimagnetic systems, concave towards the temperature axis. We have also been able to delineate regions of the (r, θ) plane characterised by distinct critical behaviour. Qualitative agreement with the exact results for $\theta = 1.0$ leads us to suppose a general validity for our results.

Acknowledgments

We wish to thank G M Bell for suggesting this problem and for useful discussions throughout its development. A G Quinn acknowledges financial support from Chelsea College.

References

- Baxter R 1975 *J. Phys. A: Math. Gen.* **8** 1797
- Baxter R J and Wu F Y 1973 *Phys. Rev. Lett.* **31** 1294
- 1974 *Aust. J. Phys.* **27** 357
- Bell G M 1974a *J. Phys. C: Solid State Phys.* **7** 1174
- 1974b *J. Phys. C: Solid State Phys.* **7** 1189
- Fisher M E 1959 *Phys. Rev.* **113** 969
- Houtappel R M F 1950 *Physica* **16** 425
- Imbro D and Hemmer P C 1976 *Phys. Lett.* **57A** 297
- Lavis D A, Southern B W and Bell G M 1982 *J. Phys. C: Solid State Phys.* **15** 1077
- Martin D H 1967 *Magnetism in Solids* (London: Iliffe)
- Néel L 1948 *Ann. Phys., Paris* **3** 137
- 1953 *Rev. Mod. Phys.* **25** 58
- Nienhuis B and Nauenberg M 1975 *Phys. Rev. Lett.* **35** 477
- den Nijs M P N, Pruisken A M M and van Leeuwen J M J 1976 *Physica A* **84** 539
- Schick M and Griffiths R B 1977 *J. Phys. A: Math. Gen.* **10** 2123
- Schick M, Walker J S and Wortis M 1977 *Phys. Rev. B* **16** 2205
- Southern B W and Lavis D A 1979 *J. Phys. C: Solid State Phys.* **12** 5333
- 1980 *J. Phys. A: Math. Gen.* **13** 251
- Szyozi I 1972 *Phase Transitions and Critical Phenomena* vol 1, ed. C Domb and M S Green (London: Academic Press)
- Wannier G H 1950 *Phys. Rev.* **79** 357
- Wolf W P 1961 *Rep. Prog. Phys.* **24** 212
- Young A P and Lavis D A 1979 *J. Phys. A: Math. Gen.* **12** 229