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Transfer matrix and phenomenological renormalisation methods applied to a triangular Ising ferrimagnetic model

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Abstract. We study a two-dimensional Ising model on a triangular lattice which is divided into two sublattices. One consists of a honeycomb of sites and the other of the remaining interstitial sites. The interaction energies within the honeycomb and between the honeycomb and the interstitial sites differ from each other. The method used consists of a combination of transfer matrix techniques and the phenomenological renormalisation procedure. Results are presented for the critical temperature and exponents in zero field and the phase diagram in the temperature–field plane is obtained.

1. Introduction

The use of transfer matrix methods in the statistical mechanics of lattice systems is well known, both as a means of obtaining the exact solution of the two-dimensional Ising model (Onsager 1944) and for obtaining approximate solutions for more complex systems (Ree and Chesnut 1966, Runnels and Combs 1966, Bellemans and Nigam 1967, Lavis 1976). In the latter context a one-dimensionally infinite lattice, with periodic boundary conditions, is used as an approximation to a two-dimensionally infinite system. Although such a system, with short-range forces, will not exhibit phase transitions, maxima in thermodynamic response functions and in the correlation length can be observed and are used to give the approximate locations of the phase transitions that would occur in the corresponding two-dimensionally infinite system.

The phenomenological renormalisation method is based on the finite-size scaling method of Fisher (1971) and Fisher and Barber (1972). It utilises the transfer matrix formalism in combination with renormalisation group procedures and was introduced by Nightingale (1976). It has now been used by many workers (Sneddon 1978, 1979, Derrida and Vannimenus 1980, Nightingale and Blöte 1980, Wood and Goldfinch 1980, Kinzel and Schick 1981, Goldfinch and Wood 1982, Droz and Malaspinas 1983) to obtain numerical estimates of second-order critical-point parameters. It has also been applied to situations where it is known that the phase transition is of first order (Blöte *et al* 1981, Roomany and Wyld 1981). Wood and Osbaldestin (1982, 1983) have argued that an inherent characteristic of the method is that it locates phase transitions without having the ability to distinguish between surfaces of critical points (second-order transitions) and coexistence surfaces (first-order transitions). This has led them to develop the method into a general procedure for obtaining an approximate form for full equilibrium phase diagrams, including the locations of points of multi-phase coexistence. We shall use both traditional transfer matrix methods and phenomenological renormalisation techniques in our investigation of the triangular ferrimagnetic Ising model, which was introduced by Bell (1974a, b) and investigated by Lavis and Quinn (1983) using a finite-cluster renormalisation group method. One characteristic property of ferrimagnets is the shape of the inverse zero-field susceptibility curve above the critical temperature. Unlike in the case of a ferromagnet, this is normally concave towards the temperature axis and the intercept of its high-temperature asymptote and the axis is 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 because of the cancellation of sublattice magnetisations. This point lies at the end of a line of first-order transitions in the temperature–field plane. Both the mean-field methods of Bell (1974a, b) and the cluster renormalisation methods of Lavis and Quinn (1983) indicate that the model under discussion is able to produce these ferrimagnetic properties. Our present results support this. They also appear to give more accurate values for critical properties.

In § 2 the model is introduced, in § 3 the methods of investigation are described, in § 4 our results are presented and in § 5 our conclusions are given.

2. The model

A triangular lattice is divided into a honeycomb sublattice b and a sublattice a consisting of the interstitial sites. The sites of sublattices a and b are occupied by ions of magnetic moments ε_a and ε_b respectively. The nearest-neighbour exchange energies are $-J_{bb}$ and $-J_{ab}$ for b–b and a–b pairs respectively. The Hamiltonian $\mathcal{H}$ is then given by

$$\mathcal{H} = \sum_{\triangle} \mathcal{H}_{\triangle} \tag{1a}$$

where

$$\mathcal{H}_{\triangle} = -(J_{ab}S_aS_{b1} + J_{ab}S_aS_{b2} + J_{bb}S_{b1}S_{b2})/2 - H(\varepsilon_a S_a + \varepsilon_b S_{b1} + \varepsilon_b S_{b2})/6 \tag{1b}$$

and the sum in (1*a*) is over all the elementary triangles of the lattice, each one consisting of an a site and two b sites, b1 and b2. The spin variables S_a, S_{b1} and S_{b2} can take the values ± 1. The six possible ground states of the system have been described in detail by Lavis and Quinn (1983). They are $\mathrm{F}^{(\pm)}$: ferromagnetic ordering with spin orientation ± 1; $\mathrm{FI}^{(\pm)}$: ferromagnetic ordering on sublattice b with spin orientation ± 1 and spin orientation ∓ 1 on sublattice a; $\mathrm{AF}^{(\pm)}$: antiferromagnetic ordering on sublattice b with the spins on sublattice a in state ± 1.

On the zero-field axis the Hamiltonian is invariant under spin inversion and the ground states will be denoted by F, FI and AF respectively. In our analysis we shall consider only $J_{ab} \leqslant 0$ and, in the case of non-zero field, we shall also restrict our attention to $J_{bb} > 0$. We use the parameters

$$\theta = |J_{ab}|/(|J_{ab}| + |J_{bb}|) \tag{2a}$$

and

$$r = \varepsilon_a/\varepsilon_b \tag{2b}$$

and the reduced temperature and field variables

$$\tilde{T} = kT/(|J_{ab}| + |J_{bb}|) \tag{2c}$$

and

$$\tilde{H} = \varepsilon_b H/(|J_{ab}| + |J_{bb}|) \tag{2d}$$

respectively, where k is Boltzmann's constant.

3. Methods

3.1. The transfer matrix method

The sites $\{\boldsymbol{R}\}$ of the triangular lattice are given, in terms of the cartesian unit vectors $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{y}}$, by

$$\boldsymbol{R} = R_0[p\hat{\boldsymbol{x}} + q(\hat{\boldsymbol{x}} + 3^{1/2}\hat{\boldsymbol{y}})/2] \tag{3}$$

where R_0 is the lattice spacing, $p = 1, 2, \ldots, N$ and $q = 1, 2, \ldots, n$ and periodic boundary conditions are applied in both directions. Because of the sublattice structure, both n and N must be integer multiples of three. The sites of the lattice with particular fixed values of p and q are called the pth column and qth row respectively.

Let $\mathcal{H}^{(p,p+1)}$ be the contribution to the Hamiltonian from the interaction between columns p and $p+1$, including half the energy of the interactions with the external field. If the spin states of a lattice column are labelled $j = 1, 2, \ldots, 2^n$ then the Boltzmann factor $\exp(-\mathcal{H}^{(p,p+1)}/kT)$ is an element of the transfer matrix $\mathbf{V}^{(n)}$, and the partition function $Z^{(n)}$ is given by

$$Z^{(n)} = \mathrm{Tr}[(\mathbf{V}^{(n)})^N] = \sum_i (\lambda_i^{(n)})^N \tag{4}$$

where $\lambda_i^{(n)}$, $i = 1, 2, \ldots, 2^n$, are the eigenvalues of $\mathbf{V}^{(n)}$, arranged in descending order of magnitude. All the elements of $\mathbf{V}^{(n)}$ are strictly positive and it follows from Perron's theorem (see, e.g., Gantmacher 1959) that $\lambda_1^{(n)}$ is real and positive with $\lambda_1^{(n)} > |\lambda_i^{(n)}|$, $i = 2, 3, \ldots, 2^n$. In the limit of large N the dimensionless free energy $\varphi_1^{(n)}$, per lattice site, is given by

$$\varphi_1^{(n)} = -(1/nN)\ln Z^{(n)} = -(1/n)\ln \lambda_1^{(n)} \tag{5}$$

and the *inverse* correlation length $\zeta^{(n)}$ is given (Domb 1960) by

$$\zeta^{(n)} = c\ln(|\lambda_1^{(n)}/\lambda_2^{(n)}|) \tag{6}$$

where c is a function only of the lattice spacing R_0. By analogy with (5) we define

$$\varphi_2^{(n)} = -(1/n)\ln|\lambda_2^{(n)}| \tag{7}$$

and it follows that

$$\zeta^{(n)} = cn(\varphi_2^{(n)} - \varphi_1^{(n)}). \tag{8}$$

In the two-dimensionally infinite version of our model ($n \to \infty$) the occurrence of a phase transition would be associated with degeneracy in the largest eigenvalue of the transfer matrix. This event, which from (6) is equivalent to a zero in the inverse correlation length $\zeta^{(\infty)}$, is usually associated with the occurrence of a second-order transition.

Kac (1968) has, however, argued that asymptotic degeneracy is a general mathematical mechanism for phase transitions and represents the appearance of two stable phases. It may, therefore, be indicative of either a second- or first-order transition. For finite n, thermodynamic functions have no singularities. We can, however, obtain estimates for phase transitions in the infinite system by locating minima in $\zeta^{(n)}$ as a function of $\tilde{T}$ at constant $\tilde{H}$, for our system with finite n, expecting our estimates to become increasingly accurate as n is increased. In the temperature–field plane the minima in $\zeta^{(n)}$ form a line of points denoted by $\mathscr{L}^{(n)}$. From (8) it will be seen that $\mathscr{L}^{(n)}$ corresponds to the line of closest approach of the values of the functions $\varphi_1^{(n)}$ and $\varphi_2^{(n)}$ at constant field. In the spirit of mean-field theory and of the argument of Kac (1968), referred to above, we could interpret $\varphi_2^{(n)}$ as the free energy of a metastable phase.

3.2. *The phenomenological renormalisation method*

The essence of the finite-size scaling method (see, e.g., Barber 1983) is the extrapolation of results for finite systems to obtain estimates for the critical properties of infinite systems. For relatively complex systems, like the one under consideration, the size of the matrices involved makes this procedure difficult to implement beyond quite small values of n. The alternative method, due to Nightingale (1976), is based on the supposition that we can define a mapping $(\tilde{T}, \tilde{H}) \to (\tilde{T}', \tilde{H}')$, in the temperature–field plane, that satisfies the relationship

$$n\zeta^{(n)}(\tilde{T}, \tilde{H}) = n'\zeta^{(n')}(\tilde{T}', \tilde{H}') \tag{9}$$

where $n' < n$. Equation (9) is not alone sufficient to define the mapping, except if $\tilde{H} = 0$, when, on symmetry grounds, we must have $\tilde{H}' = 0$. The zero-field axis is, therefore, an invariant subspace of the transformation. Let $(\tilde{T}_0, 0)$ be a fixed point and define $t = \tilde{T} - \tilde{T}_0$. We now express (9) in the form

$$\zeta^{(n')}(tb^{x_T}, \tilde{H}b^{x_H}) = b\zeta^{(n)}(t, \tilde{H}) \tag{10}$$

where $b = n/n'$ and we have defined the exponents x_T and x_H according to the formulae

$$t' = tb^{x_T} \tag{11a}$$

$$\tilde{H}' = \tilde{H}b^{x_H}. \tag{11b}$$

Equation (10) is very similar to the scaling equation

$$\zeta(\tau b^{y_T}, \tilde{H}b^{y_H}) = b\zeta(\tau, \tilde{H}) \tag{12}$$

for the inverse correlation length ζ of the two-dimensionally infinite system, where $\tau = \tilde{T} - \tilde{T}_c$, $\tilde{T}_c$ being the critical temperature of the infinite system. Nightingale's method is based on the hypothesis that (10) is an approximation to (12), which becomes increasingly accurate as $n, n' \to \infty$ with b remaining finite. This assumes the convergence of the limiting procedures $\tilde{T}_0(b, n) \to \tilde{T}_c$, $x_T(b, n) \to y_T$, $x_H(b, n) \to y_H$ and $\zeta^{(n)} \to \zeta^{(\infty)} = \zeta$. Numerical calculations for the two-dimensional Ising model (Nightingale 1976) provide strong support for this conjecture. They show that, although the rate of convergence is affected by the relationship between n and n', it is achieved for a variety of choices, with the optimum strategy being

$$n' = n - p_0 \tag{13}$$

where p_0 is the periodicity of the system ($p_0 = 1$ for the simple ferromagnetic Ising model, $p_0 = 3$ for our system).

An important aspect of phenomenological renormalisation is that it is able to yield numerical estimates x_T and x_H for the values of the critical exponents y_T and y_H. This contrasts with scaling theory, of which (12) is a part, which gives the scaling law relationships between exponents (see, e.g., Hankey and Stanley 1972), but no numerical values for the individual exponents. Following Wood and Osbaldestin (1982) we define the function

$$\psi^{(n)}(T, H) = n'\zeta^{(n')}(\tilde{T}, \tilde{H}) - n\zeta^{(n)}(\tilde{T}, \tilde{H}). \tag{14}$$

It will then be seen that a solution $\tilde{T} = \tilde{T}_0$ of the equation

$$\psi^{(n)}(\tilde{T}, 0) = 0 \tag{15}$$

will correspond to the fixed point $(\tilde{T}_0, 0)$ of the mapping defined by (9), when n' is given by (13). Having found $\tilde{T}_0$, which is taken to be our estimate of the critical temperature $\tilde{T}_c$, the exponent x_T is given, from (10), by

$$x_T = \ln[(\partial\zeta^{(n)}/\partial\tilde{T})_0/(\partial\zeta^{(n')}/\partial\tilde{T})_0]/\ln(n/n') + 1 \tag{16}$$

where the subscript 0 indicates that the derivatives are evaluated at the fixed point. A similar procedure can be adopted for the evaluation of x_H, except that, since $\zeta^{(n)}$ and $\zeta^{(n')}$ are even functions of $\tilde{H}$, we must use the second derivative of (10). This gives

$$x_H = \ln[(\partial^2\zeta^{(n)}/\partial\tilde{H}^2)_0/(\partial^2\zeta^{(n')}/\partial\tilde{H}^2)_0]/2\ln(n/n') + \tfrac{1}{2}. \tag{17}$$

For the model of interest in this paper, first-order transitions are expected in regions of the temperature–field plane away from the zero-field axis. The method used to determine their approximate location follows the work of Wood and Osbaldestin (1982). They have argued that the solution curve $\mathscr{C}^{(n)}$ of the equation

$$\psi^{(n)}(\tilde{T}, \tilde{H}) = 0 \tag{18}$$

in the temperature–field plane converges, as n increases, on any phase equilibrium curve and that, for any finite n, $\mathscr{C}^{(n)}$ bounds a region containing all the phase equilibrium curves. At a point on $\mathscr{C}^{(n)}$ we define the exponent

$$x(\alpha) = \ln(\nabla\zeta^{(n)}\cdot\hat{\alpha}/\nabla\zeta^{(n')}\cdot\hat{\alpha})/\ln(n/n') + 1 \tag{19}$$

where the gradient is taken with respect to $(\tilde{H}, \tilde{T})$ and $\hat{\alpha} = (\cos\alpha, \sin\alpha)$. In general this exponent is a function both of α, the angle of directional differentiation with respect to the field axis, and of $\tilde{T}$ and $\tilde{H}$. Since from (14)

$$\nabla\psi^{(n)} = n'\nabla\zeta^{(n')} - n\nabla\zeta^{(n)} \tag{20}$$

it follows that, if $\hat{\alpha}$ is tangential to $\mathscr{C}^{(n)}$, then $x(\alpha) = 0$. This marginal exponent along the curve is to be expected since each point of $\mathscr{C}^{(n)}$ is a fixed point of the renormalisation transformation.

The only case in which $x(\alpha)$ does not vary with α is when the vectors $\nabla\zeta^{(n)}$ and $\nabla\zeta^{(n')}$ are parallel and, from (20), in the normal direction to $\mathscr{C}^{(n)}$. According to the argument of Kinzel and Schick (1981) this is the case that yields the value closest to the relevant exponent for the phase boundary of the system when $n \to \infty$.

4. Results

4.1. $\tilde{H} = 0$

The root $\tilde{T}_0$ of equation (15) is our approximation to the critical temperature $\tilde{T}_c$. Both $\tilde{T}_0$ and $\tilde{T}_c$ are functions of θ and the sign of J_{bb}, but not of r or of the sign of J_{ab}. We have calculated $\tilde{T}_0$ as a function of θ for $n = 6$ and $n' = 3$ and the results are presented in figure 1. Since we have taken $J_{ab} \leqslant 0$ the transition is to the phase with ground state FI in all cases shown except when $J_{bb} < 0$ and $0 < \theta < 0.5$ when the transition is to the phase with ground state AF. Our calculations can be compared with exact results in a number of special cases (see Lavis and Quinn 1983). For $\theta = 0.5, J_{bb} > 0, \tilde{T}_c = 2/\ln(3) = 1.821$, the value for the ferromagnetic isotropic Ising model, and our result is $\tilde{T}_0 = 1.822$. For $\theta = 0$ the critical temperature is that of the Ising honeycomb model, $\tilde{T}_c = 2/\ln(2 + \sqrt{3}) = 1.519$, compared with our result $\tilde{T}_0 = 1.511$. The exact critical temperature for $\theta = 1.0$ can be obtained by using a de-decoration transformation to map the model on to the isotropic ferromagnet. This yields

$$\tilde{T}_c = 2\left[\ln\left(\frac{1 + 3^{1/2} + [2(3^{1/2})]^{1/2}}{2}\right)\right]^{-1} = 2.405 \qquad (21)$$

compared with the result $\tilde{T}_0 = 2.395$ obtained here.

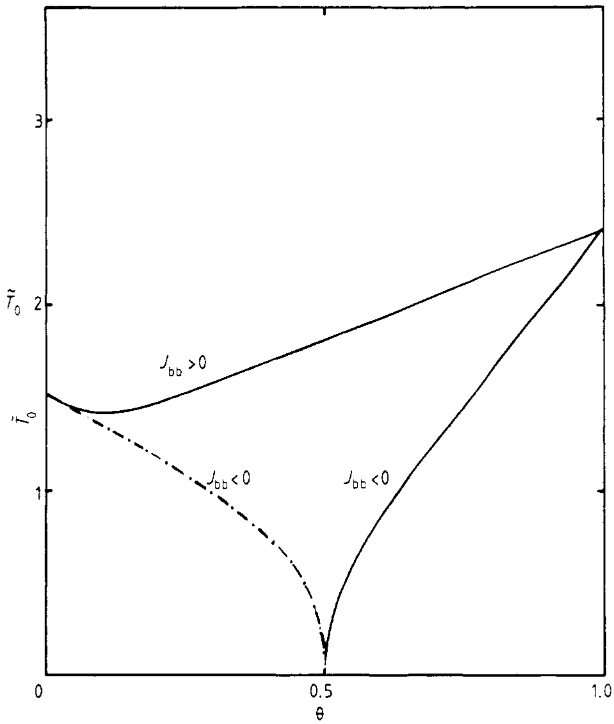

Figure 1. The critical temperature as a function of θ. The full curve represents a transition to a phase with ferrimagnetic ground state FI and the chain curve a transition to a transition to a phase with antiferromagnetic ground state AF.

For $\tilde{H}=0$ the model is isomorphic to the corresponding ferromagnetic model obtained by changing the sign of J_{ab}. This latter model is in the universality class of the isotropic ferromagnet ($J_{ab}=J_{bb}>0$) and thus for the thermal exponent we must have $y_T=1.0$. Our calculated estimate x_T for y_T shows a small variation with θ, the minimum value being 0.984 at $\theta=0$ and 1.0 and the maximum being 1.0035 at $\theta=0.5$. This latter value is the same as that derived by Kinzel and Schick (1981) for the equivalent ferromagnetic model. As may be expected, exact agreement between the results for ferromagnetic and ferrimagnetic models does not occur in the case of the magnetic exponent. As indicated in § 1, an important feature of ferrimagnetic systems is the occurrence of a compensation temperature below the critical temperature at which spin cancellation leads to a zero magnetisation. In our model this compensation temperature is a function of r and θ and is denoted by $T^*(r, \theta)$. We now denote by $r^*(\theta)$ the value of r, for some θ, at which the critical and compensation temperatures coincide. Exact results (see Lavis and Quinn 1983) indicate that, for our model, the magnetic exponent y_H should take its ferromagnetic Ising value of 1.875. However, when $r=r^*$, leading amplitudes in the thermodynamic functions are zero and the critical exponents differ from their ferromagnetic values. We have investigated the value of x_H for both ferromagnetic and ferrimagnetic cases. In the former case this exponent exhibits only a small variation with respect to θ and none with respect to r. Our results agree with the value 1.8738 obtained by Kinzel and Schick (1981) for the case where $\theta=0.5$. For the ferrimagnetic model there is a variation of x_H both with respect to θ and r. This variation is shown in figure 2, where graphs are presented for $\theta=0.0$, 0.5 and 1.0. Minima in these curves occur for $\theta=0.5$ and 1.0 at $r=2.0$ and 1.73 respectively. These values can be compared with the exact results (see Lavis and Quinn 1983) $r^*(0.5)=2.0$ and $r^*(1.0)=1.728$; which are the values of r for which the critical exponents deviate from their Ising ferromagnetic values.

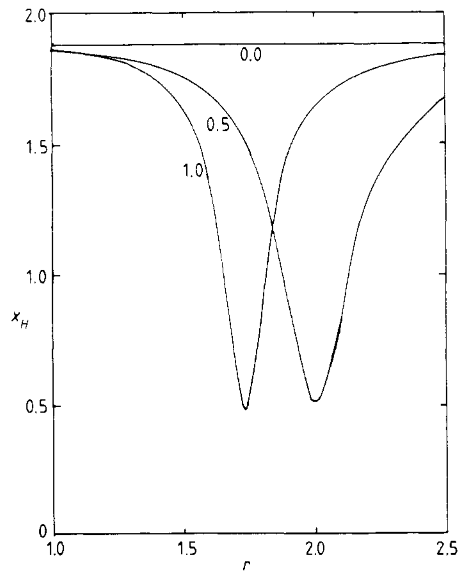

Figure 2. The variation of the estimated magnetic exponent x_H with respect to r. Curves are labelled with their values of θ.

4.2. $\tilde{H} \neq 0$

As indicated in § 2, we use both transfer matrix and phenomenological renormalisation methods to obtain the phase diagram. Results are presented in figure 3 for the case where $\theta = 1.0$ and $r = 1.9$. The broken curve in figure 3 corresponds to the curve $\mathscr{L}^{(6)}$ of minima of $\zeta^{(6)}(\tilde{T}, \tilde{H})$ with respect to $\tilde{T}$ and the full curve corresponds to the curve $\mathscr{C}^{(6)}$, obtained from (18). $\mathscr{L}^{(6)}$ can be regarded as an approximation to the first-order transition between the ferrimagnetic phases $\mathrm{FI}^{(+)}$ and $\mathrm{FI}^{(-)}$ and the intersection of $\mathscr{L}^{(6)}$ and $\mathscr{C}^{(6)}$ at $\tilde{T} = 0.747$, $\tilde{H} = 2.763$ is taken as an estimate for the end-point of the curve. Since $\zeta^{(6)}$ is monotonic on the zero-field axis, $\mathscr{L}^{(6)}$ does not meet this axis but approaches it closely after attaining a maximum temperature value of $\tilde{T} = 1.646$. This can be compared with the exact value $T^*(1.9, 1.0) = 1.658$ for the compensation temperature, which can be derived from formulae given by Lavis and Quinn (1983). The exponent $x(\alpha)$, given by (19), was calculated at various points on $\mathscr{C}^{(6)}$. On the lower branch of the curve the exponent showed a strong dependence on α, corresponding to a large angle between the vectors $\nabla\zeta^{(3)}$ and $\nabla\zeta^{(6)}$ (e.g. 0.50 rad at $\tilde{H} = 0.75$). The same was true on the upper branch of the curve from the critical point to about $\tilde{H} = 0.5$. On the remaining part of the upper branch of the curve the α-dependence of the exponent was modest other than for directions near to the tangent lines to $\mathscr{C}^{(6)}$. Two cases in this category are shown in figure 4. The corresponding angles between $\nabla\zeta^{(3)}$ and $\nabla\zeta^{(6)}$ are (A) 0.0086 rad and (B) 0.0087 rad. The fact that in case A the exponent is close to 2.0 is significant since the value expected for the relevant exponent along a first-order transition curve is $d = 2$.

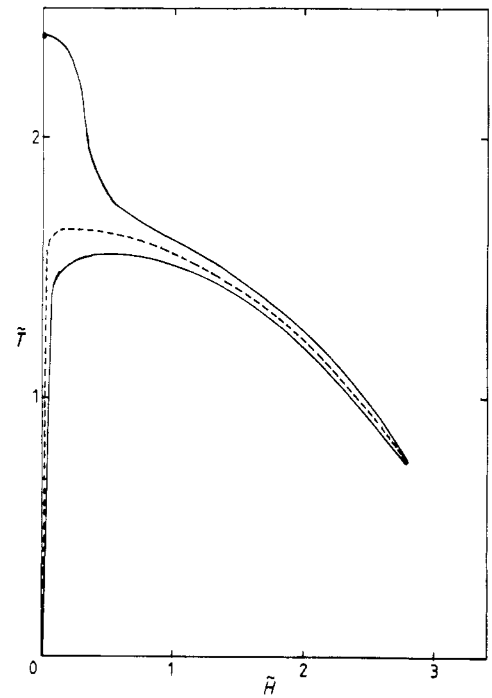

Figure 3. The phase diagram in the temperature–field plane for $\theta = 1.0$ and $r = 1.9$. The full curve corresponds to the curve $\mathscr{C}^{(6)}$ and the broken curve corresponds to the curve $\mathscr{L}^{(6)}$.

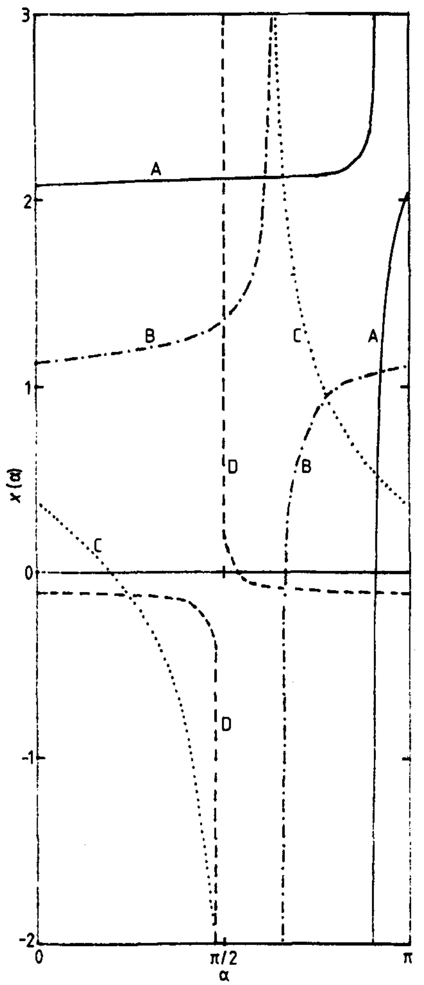

Figure 4. The variation of the exponent $x(\alpha)$ with respect to α at points (A): $\tilde{H} = 1.0$, $\tilde{T} = 1.6083$; (B) $\tilde{H} = 2.76$, $\tilde{T} = 0.7586$; (C) $\tilde{H} = 2.7628$, $\tilde{T} = 0.7471$; (D) $\tilde{H} = 2.76$, $\tilde{T} = 0.7465$ on the curve $\mathscr{C}^{(6)}$.

Case C in figure 4 corresponds to the calculated end-point of the line of first-order transitions. Here the angle between $\nabla\zeta^{(3)}$ and $\nabla\zeta^{(6)}$ is large (0.380 rad). This point lies on $\mathscr{C}^{(6)}$ between the points corresponding to cases B and D, where the α-dependence of the exponent is more modest. It may be supposed that the behaviour of the exponent in case C, as contrasted to cases B and D, is related to the existence of two relevant exponents at the end-point in the corresponding two-dimensionally infinite system.

5. Conclusions

We have investigated a two-dimensional ferrimagnetic Ising model using a combination of transfer matrix and phenomenological renormalisation methods. On the zero-field axis the critical temperature has been calculated as a function of the parameter θ. The maximum error shown for the three cases for which the exact result is known is 0.53%. The maximum error for the thermal exponent y_T at the critical point is 3.5%. Exact calculations show that the critical exponents differ from their ferromagnetic values when the critical and compensation temperatures coincide. We have demonstrated that our estimate x_H for the magnetic exponent y_H attains a minimum at this value of r. It is reasonable to suppose that, as n increases, this minimum will steepen to a point discontinuity. To predict the known value of β (see Lavis and Quinn 1983) the discontinuity value would need to be 0.875 as compared with the approximate value of 0.5 obtained here.

The qualitative features of our phase diagram are consistent with the known properties of the system and the error in our estimate of the compensation temperature is less than 0.1%. The critical exponent for the phase transition curve is close to its first-order value. Exponents in a neighbourhood of the critical end-point are more difficult to interpret.

Acknowledgments

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