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High-field expansions for the anisotropic Ising model

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Abstract. We obtain high-field series expansions for the anisotropic Ising model on a simple cubic lattice. These series are used to investigate the tricritical point that occurs when the model is used to represent metamagnets. Some new tests of scaling theory for the crossover between two and three dimensions are also undertaken.

1. Introduction

The anisotropic Ising model on a simple cubic lattice has been studied by many workers; an overall summary is included in the review by Stanley (1974). The investigations have concentrated on two general properties that are exhibited by this system: crossover between two-dimensional and three-dimensional behaviour and, for negative interlayer couplings, the tricritical point in the field–temperature plane. We have obtained new series expansions which we use to extend both these lines of investigation.

The crossover between two and three dimensions is predicted to follow the scaling theory proposed by Abe (1970) and Mikulinskii (1971). The predictions of scaling theory have been extensively tested by Krasnow *et al* (1973). Scaling theories are now interpreted in terms of the renormalization group approach pioneered by Wilson (1971a, b) with crossover phenomena arising from the competition between two fixed points of the renormalization transformation (see the review by Fisher 1974). The initial application of renormalization group techniques to the anisotropic Ising model was by Grover (1973).

There have been several studies of the case of negative interlayer coupling but for reasons of mathematical convenience these have been confined to the case when the interlayer coupling has the same magnitude as the intralayer coupling. Guttman (1972) analysed the zero-field susceptibility (using the series of Oitmaa and Enting 1972) to test the smoothness postulate (Griffiths 1970, 1971) which predicts that the susceptibility should behave in a manner similar to the internal energy. The other important property of systems with negative interlayer coupling is that an increase in the applied field changes the transition from continuous to first order, the two regimes being separated by a tricritical point. Harbus and Stanley (1972, 1973b) have investigated this type of behaviour in the anisotropic Ising model. An example of an 'Ising' system showing such metamagnetic behaviour is $FeCl_2$ (Birgeneau *et al* 1974).

We have obtained low-temperature series for the anisotropic Ising model described by Hamiltonian (2.1), by generalizing the method of partial generating functions (the code method) of Sykes *et al* (1965). From the low-temperature or high-field series, the low-temperature to high-temperature transformation of Domb (1949) gives high-temperature series for the general field free energy. The high-field series and the high-temperature series are complete to ninth order in the appropriate expansion variables. Longer series are available for special cases as discussed in § 2. The main restriction is that we do not have series expansions for particular correlation functions (cf Stanley and co-workers, unpublished) so that we can investigate neither moments of correlation functions (cf Harbus and Stanley 1973a, Krasnow *et al* 1973) nor staggered susceptibilities (cf Harbus and Stanley 1972, 1973b).

The anisotropic Ising model, its parameter space and the possible types of series expansion are described in § 2. Then § 3 describes the generalization of the method of partial generating functions; § 4 describes transformations of the general series into forms suitable for conventional series analysis techniques. In § 5 the scaling theory of the two-dimensions to three-dimensions crossover is described and some new tests of the theory are described, in particular the approach to the square lattice critical point along the critical isotherm. In § 6 the new series is used to extend the investigation of the tricritical point begun by Harbus and Stanley (1972, 1973b) and an estimate of the tricritical magnetization is obtained. Then § 7 concludes the paper with a discussion of the reasons for the power and utility of the series derivation techniques used.

2. The anisotropic Ising model

The model that we consider is defined on a simple cubic lattice of N sites $\boldsymbol{r}_i$ by the Hamiltonian

$$\mathscr{H} = -\sum_{(\boldsymbol{r}_i,\boldsymbol{r}_j)} J(\boldsymbol{r}_i-\boldsymbol{r}_j)\sigma(\boldsymbol{r}_i)\sigma(\boldsymbol{r}_j) - \sum_{\{\boldsymbol{r}_i\}} H\sigma(\boldsymbol{r}_i) \tag{2.1}$$

where

$$J(\boldsymbol{r}_i-\boldsymbol{r}_j) = \begin{cases} J & \text{if } \boldsymbol{r}_i, \boldsymbol{r}_j \text{ are neighbours in the same } x\text{–}y \text{ plane} \\ \eta J & \text{if } \boldsymbol{r}_i, \boldsymbol{r}_j \text{ are neighbours in adjacent } x\text{–}y \text{ planes} \\ 0 & \text{otherwise.} \end{cases}$$

The Ising spin variables take the values $\sigma(\boldsymbol{r}_i) = \pm 1$. The first sum in (2.1) sums over each pair only once.

The general behaviour of the anisotropic Ising model in a uniform field is indicated in figure 1.

There are three phase transition surfaces:

A. $H=0$, $\eta>0$, $T<T_{\mathrm{D}}(\eta)$
This is a surface of first-order transitions with a discontinuous change in magnetization across the surface, bounded by a line of critical points. $T=T_{\mathrm{D}}(\eta)$ is discussed under D below.

B. $\eta<0$, $T=T_{\mathrm{B}}(H,\eta)$, $H_{\mathrm{t}}(\eta)<|H|<-2\eta$
This is also a surface of first-order transitions separating phases with a uniform layer magnetization from systems with a staggering of the layer magnetizations. The function $H_{\mathrm{t}}(\eta)$ is discussed under E below. Apart from the smooth curve sketched by Harbus and Stanley (1972) to represent $T_{\mathrm{B}}(H,-1)$, $T_{\mathrm{B}}(H,\eta)$ has not been investigated.

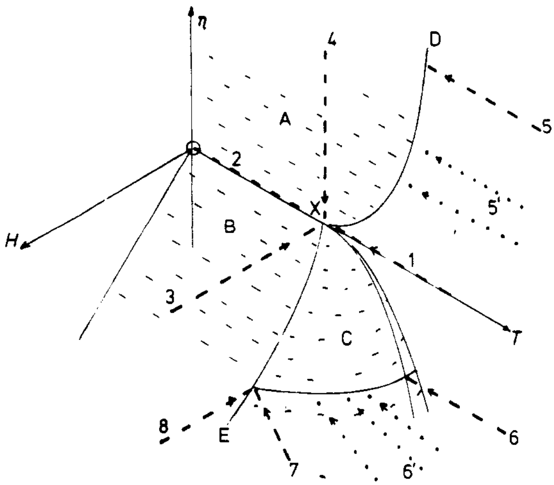

Figure 1. The transition surfaces of the anisotropic Ising model. A and B are surfaces of first-order transitions and C is a surface of critical points. D is a line of critical points and E is a line of tricritical points. X is the square lattice Ising model critical point. Lines 1 to 8 are trajectories along which the standard analysis techniques for single-variable series can be used.

C. $\eta < 0, |H| < H_t(\eta), T = T_C(H, \eta)$
This is a surface of continuous transitions separating regions of uniform layer magnetization from regions of staggered layer magnetization. The line $T_C(H, -1)$ was investigated by Harbus and Stanley (1972, 1973b). Symmetry considerations show that $T_C(0, -\eta) = T_D(\eta), \eta > 0$.

These surfaces have two special boundary lines:

D. $H = 0, \eta > 0, T = T_D(\eta)$
The location of this line was investigated by Paul and Stanley (1972), Oitmaa and Enting (1972) and Enting (1973b). The behaviour of the series results agreed with universality theory and had a crossover behaviour as predicted by scaling theories.

E. $\eta < 0, H = \pm H_t(\eta), T = T_t(\eta)$
This line separates surface B from surface C so that:

$$T_t(\eta) = \lim_{|H| \to H_t(\eta)^+} T_B(H, \eta) = \lim_{|H| \to H_t(\eta)^-} T_C(H, \eta).$$

This line (or rather pair of lines for positive and negative H) is a line of tricritical points. The Harbus and Stanley estimates of $T_t(-1)$, $H_t(-1)$ are given in § 6.

X. Finally there is the point X of figure 1 which is the two-dimensional Ising critical point $H = \eta = 0, T = T_I = J/(k \tanh^{-1}(\sqrt{2} - 1))$.

When the conventional techniques of analysis (Gaunt and Guttmann 1974) are used they require that the expressions be in terms of one variable so that series investigations of the anisotropic Ising model are defined along particular lines in the parameter space shown in figure 1. The present investigation and previous investigations can thus be classified in terms of such lines.

Line 1. $\eta = H = 0, T > T_I$
Without any η dependence this line is the zero-field square lattice Ising model for which

extensive series investigations have been undertaken (Domb 1974). Derivatives with respect to η of the susceptibility, specific heat and moments of the correlation function were investigated by Krasnow *et al* (1973). In § 5 we consider one additional derivative.

Line 2. $\eta = H = 0$, $T < T_{\mathrm{I}}$
Again for the two-dimensional Ising model extensive series investigations have been performed. Although our series apply to this region, in practice they are too short for useful tests of crossover scaling.

Line 3. $\eta = 0$, $T = T_{\mathrm{I}}$
This is the critical isotherm of the square lattice Ising model. The behaviour of the magnetization was first investigated by Gaunt *et al* (1964). Betts and Filipow (1972) investigated two-parameter scaling theory. In § 5 we give the first tests of three-parameter crossover scaling theory along the critical isotherm.

Line 4. $H = 0$, $T = T_{\mathrm{I}}$, $\eta > 0$
On the FCC lattice the large-η region corresponds to a BCC lattice model so that large-η expansions can be obtained by expanding about an ordered state. Enting (1974) tested the three-parameter scaling hypothesis along the line $\eta \to 0$ for the anisotropic FCC lattice. On the simple cubic the large-η regime corresponds to the one-dimensional Ising model and so the large-η expansions of Citteur and Kasteleyn (1972, 1973a, b) and Citteur (1973a, b) are more closely related to high-temperature expansions.

Line 5. $H = 0$, $\eta = 1$
This is the simple cubic Ising model. Again extensive series investigations have been undertaken (see Domb 1974).

Class 5. $H = 0$, η fixed
These lines were investigated by Paul and Stanley (1972) and Oitmaa and Enting (1972). Susceptibility series were used to obtain estimates of $T_{\mathrm{D}}(\eta)$. These susceptibility series are longer than those obtained in the present work (note the minor corrections given by Oitmaa and Enting 1975). Universality theory predicts that the behaviour along all lines in this class shall have behaviour similar to line 5.

Line 6. $\eta = -1$, $H = 0$
The susceptibility along this line was investigated by Guttmann (1972) to test the smoothness postulate which predicts that the susceptibility will behave as the internal energy along all lines in class 6′. Many properties on this line are by symmetry equivalent to those on line 5.

Class 6′. $\eta = -1$ fixed, $H/T < H_{\mathrm{t}}(-1)/T_{\mathrm{t}}(-1)$
Harbus and Stanley (1972, 1973b) used staggered susceptibility series along these lines to locate the line $T_{\mathrm{C}}(H, -1)$. They also give susceptibility series appropriate to these lines. In § 4 we extend the susceptibility series by an additional term in the temperature variable (as a polynomial in the field variable) and remove the numerical uncertainties from the Harbus and Stanley coefficients. Since we lack series for the staggered susceptibility we cannot refine their estimates of $T_{\mathrm{C}}(H, -1)$.

Line 7. $\eta = -1$, $H/T = H_{\mathrm{t}}(-1)/T_{\mathrm{t}}(-1)$
We use our extended susceptibility series to extend the analysis of the tricritical point begun by Harbus and Stanley.

Line 8. $\eta = -1$, $T = T_t(-1)$, $H > H_t(-1)$
This is the tricritical isotherm. In § 6 we find that the series are too irregular to give useful results in our new test of tricritical scaling. On the basis of scaling theory we can however estimate the tricritical magnetization.

3. High-field series

The free energy F is obtained from the Hamiltonian $\mathscr{H}$ by means of the relation

$$F(T, H, \eta) = -\frac{1}{N} kT \ln\left(\sum_{\sigma \text{ states}} \exp(-\mathscr{H}/kT)\right) \tag{3.1}$$

where k is Boltzman's constant. We define the reduced free energy $\ln \Lambda$ and its low-temperature–high-field expansion by

$$\begin{aligned} \ln \Lambda &= -F(T, H, \eta)/kT + \lim_{T \to 0} F(T, H, \eta)/kT \\ &= \sum a_{mnp} u^m v^n \mu^p = \sum L_m(u, v) \mu^m \end{aligned} \tag{3.2}$$

where

$$u = \exp(-4J/kT) \tag{3.3a}$$

$$v = \exp(-4\eta J/kT) \tag{3.3b}$$

$$\mu = \exp(-2H/kT). \tag{3.3c}$$

The $L_m(u, v)$ are polynomials of degree $2m$ in u and m in v. The series are derived by a simple generalization of the method of Sykes *et al* (1965) which divides the simple cubic lattice into two equivalent sublattices A and B so that any pair of neighbours lies one on each sublattice. The field H is generalized to H_A on lattice A and H_B on lattice B so that μ generalizes to μ_A and μ_B and (3.2) becomes

$$\ln \Lambda = \sum_{mn} L_{mn}(u, v) \mu_A^m \mu_B^n. \tag{3.4}$$

The power of the method comes from two properties:

(i) $$L_{mn}(u, v) = L_{mn}(u, v) \tag{3.5}$$

(ii) for small m it is possible to obtain closed form expressions for F_m defined by

$$\sum_{n \geq 0} L_{mn}(u, v) \mu^n = u^{2m} v^m F_m(u, v, \mu). \tag{3.6}$$

The F_m which are known as partial generating functions are traditionally represented in a coded form $\Sigma\, C_i(\lambda; \alpha, \beta; \gamma, \delta, \epsilon; \ldots)$ where the expression $(\lambda; \alpha, \beta; \gamma, \delta, \epsilon; \ldots)$ represents $f_0^{-\lambda} f_1^{\alpha} f_2^{\beta} f_3^{\gamma} \ldots$. Our notation departs from that of Sykes *et al* (1965) by our use of semicolons to group together sets of coefficients that would be combined in the simple cubic case. The F_m, $0 \leq m \leq 4$, are given in the appendix.

The f_i are

$$f_0 = 1 + \mu u^2 v \tag{3.7a}$$

$$f_1 = 1 + \mu u v \tag{3.7b}$$

$$f_2 = 1+\mu u^2 \tag{3.7c}$$
$$f_3 = 1+\mu v \tag{3.7d}$$
$$f_4 = 1+\mu u \tag{3.7e}$$
$$f_5 = 1+\mu u^2 v^{-1} \tag{3.7f}$$
$$f_6 = 1+\mu u^{-1} v \tag{3.7g}$$
$$f_7 = 1+\mu \tag{3.7h}$$
$$f_8 = 1+\mu u v^{-1} \tag{3.7i}$$
$$f_9 = 1+\mu u^2 v^{-2} \tag{3.7j}$$
$$f_{10} = 1+\mu u^{-2} v \tag{3.7k}$$
$$f_{11} = 1+\mu u^{-1} \tag{3.7l}$$
$$f_{12} = 1+\mu v^{-1} \tag{3.7m}$$
$$f_{13} = 1+\mu u v^{-2} \tag{3.7n}$$
$$f_{14} = 1+\mu u v^{-3}. \tag{3.7o}$$

When the F_m are expanded we recombine the series using

$$L_n(u, v) = \sum_{m=0}^{n} L_{m,n-m}(u, v). \tag{3.8}$$

The symmetry property (3.5) means that F_0 to F_4 are sufficient to give series for L_1 to L_9. These series are given in the appendix.

There are a number of checks on the manipulations of these series. The symmetry property (3.5) provides one such check. In addition the coded partial generating functions can be combined to give the partial generating functions for the isotropic cases (SQ and SC) tabulated by Sykes *et al* (1965). Similarly the final series can be combined to give series for the isotropic cases giving a test both of the expressions F_m and the expansion procedure. Another more powerful test comes from the low-temperature–high-temperature transformation used in the next section. The results of this transformation must agree with series such as the susceptibility series of the anisotropic Ising model and the general field series for $\eta = -1$.

The high-field series given in the appendix can be used directly for two of the cases considered in § 2. For the square lattice critical isotherm, simple substitution of $u = (\sqrt{2}-1)^2$, $v = 1$ after taking appropriate derivatives gives the series used in § 5 for investigating gap exponents.

Similarly to investigate the approach to the $\eta = -1$ tricritical point along line 8 of figure 1 we use $u = \exp(-4J/kT_t)$, $v = u^{-1}$.

4. High-temperature expansions

The high-temperature expansion of the free energy has the form

$$F(T, H, \eta) = 2 \ln \cosh(J/kT) + \ln \cosh(\eta J/kT) + \ln \cosh(H/kT) + \sum_{mnp} a_{mnp} w_1^m w_2^n x^p \tag{4.1}$$

where

$$w_1 = \tanh(J/kT) \tag{4.2a}$$

$$w_2 = \tanh(\eta J/kT) \tag{4.2b}$$

$$x = \tanh^2(H/kT) \tag{4.2c}$$

and

$$a_{mnp} = 0 \qquad \text{if } p > m + n. \tag{4.3}$$

Domb (1949) pointed out that such high-temperature expansions can be obtained from low-temperature expansions. We give a transformation formalism without proof.

Consider

$$\ln \Lambda = \sum L_m(u, v)\mu^m$$

and substitute

$$u = (1-w_1)^2/(1+w_1)^2 \tag{4.4a}$$

$$v = (1-w_2)^2/(1-w_2)^2 \tag{4.4b}$$

to give

$$\ln \Lambda = \sum \bar{L}_m(w_1, w_2)\mu_m = \sum \bar{a}_{mnp} w_1^m w_2^n \mu^p. \tag{4.5}$$

This will give $\bar{L}_m$ as an infinite series in w_1, w_2 but for the purposes of what follows this series can be truncated after terms $w_1^a w_2^b$ where $a + b = M$, the maximum m value for which L_m is known (nine in the present work).

Comparing the coefficients of $w_1^m w_2^n$ in (4.1) and (4.5) gives

$$\sum_p a_{mnp}(1-\mu)^{2p}/(1+\mu)^{2p} = \sum_p \bar{a}_{mnp}\mu^p \qquad m, n \neq 0. \tag{4.6}$$

The ten known $\bar{a}_{mnp}$ (including $\bar{a}_{mn0} = 0$) are sufficient to determine the $m + n + 1$ non-zero a_{mnp} for $m + n \leq 9$. Equation (4.6) is simply a set of linear equations in the unknowns a_{mnp}. If either m or n is zero additional terms from the ln cosh terms and the $T \to 0$ limit occurring in (3.2) occur in equation (4.6). To test our transformation we checked our series for the isotropic cases against the series used by Essam and Hunter (1968) (series from Essam, private communication).

The general series is not given here because of its considerable length. We have only used it to obtain the series for $(\partial^4/\partial H^4)(\partial/\partial\eta)F$ analysed in the following section and to extend the Harbus and Stanley susceptibility series.

In connection with the $\eta = -1$ case it should be noted that one can fix $\eta = -1$, i.e. $v = u^{-1}$, $w_2 = -w_1$, *before* performing the low–high transformation from series in u, μ to series in w_1, x. In fact the substitution $v = u^{-1}$ can be performed before expanding the partial generating functions F_m. Alternatively one could perform the substitutions $u = (1-w_1)^2/(1+w_1)^2$, $v = (1+w_1)^2/(1-w_1)^2$ *before* expanding the F_m, truncating the series at the appropriate order. We have not however investigated the efficiency of such an approach.

Using $\chi = -\partial^2 F/\partial H^2$ gives

$$\chi kT = 1 - x + \sum_{mn} b_{mn0} w_1^m w_2^n [2p(2p+1)x^{p+1} - 8p^2 x^p + 2p(2p-1)x^{p-1}]. \tag{4.7}$$

For $\eta = -1$ this sums to give

$$\chi kT = \sum_{n=0}^{\infty} w_1^n a_n(x) \tag{4.8}$$

where the $a_n(x)$ are polynomials of degree n in x given for $n \leq 8$ by Harbus and Stanley (1972). We have been able to remove the numerical uncertainty from their coefficients a_8 and give a_9 for the first time:

$$a_8 = -1402 - 28478x + 1155680x^2 - 10011488x^3 + 40107912x^4 - 88872520x^5 + 115745632x^6 - 88314336x^7 + 36561938x^8 - 6342938x^9$$

$$a_9 = -3214 + 96472x + 294622x^2 - 15005504x^3 + 112019260x^4 - 400902768x^5 + 819495364x^6 - 1008092992x^7 + 739554500x^8 - 298567792x^9 + 51112052x^{10}.$$

5. Tests of scaling theory

The content of the crossover scaling theory proposed by Abe (1970) and Mikulinskii (1971) can be condensed into the form given by Hankey and Stanley (1972) who make the basic assumption that G, the singular part of the free energy F can be written as a generalized homogeneous function sufficiently near the critical point

$$\lambda G(\epsilon, H, \eta) = G(\lambda^a \epsilon, \lambda^b H, \lambda^c \eta) \tag{5.1}$$

where

$$\epsilon = T - T_1. \tag{5.2}$$

Defining

$$G_{pqr} = \left(\frac{\partial}{\partial \epsilon}\right)^p \left(\frac{\partial}{\partial H}\right)^q \left(\frac{\partial}{\partial \eta}\right)^r \tag{5.3}$$

assumption (5.1) predicts that the singular part of G_{pqr} behaves as

$$G_{pqr} \sim \begin{cases} |\epsilon|^{y/a}, & \epsilon \to 0, H = \eta = 0 \quad (5.4a) \\ |H|^{y/b}, & H \to 0, \epsilon = \eta = 0 \quad (5.4b) \\ |\eta|^{y/c}, & \eta \to 0, \epsilon = H = 0 \quad (5.4c) \end{cases}$$

$$y = 1 - pa - qb - rc. \tag{5.5a}$$

The exact solutions for the square lattice Ising model require $a = \frac{1}{2}$, $b = \frac{15}{16}$. Realizing that for $\eta = H = 0$, G_{001}, the interlayer correlation function, is proportional to the square of the magnetization G_{010}, assumption (5.1) requires

$$2(1-b)/a = (1-c)/a \tag{5.5b}$$

or $c = \frac{7}{8}$. The renormalization group approach provides a justification of assumption (5.1) and approximate realizations of the renormalization transformation can lead to predictions for a, b and c.

When the scaling hypothesis (5.1) is combined with the assumption of two-parameter scaling along the line $T_D(\eta)$, the theory predicts the behaviour of critical amplitudes as $\eta \to 0$ and the shape of the $T_D(\eta)$ curve. The scaling prediction of the exponent describing $T_D(\eta)$ is equal to the value of the bound found by Enting (1973a).

For $\epsilon \to 0$ the behaviour predicted by equation (5.4a) has been tested by investigations of series for G_{20m} and G_{02m} for small m. This work has been described by Krasnow *et al* (1973) and Stanley (1974) who also give a number of exact results. They also investigated moments of correlation functions.

We have used the high-temperature series to investigate G_{041} and having constructed Padé approximants we obtain exponent estimates

$$G_{041} \sim \epsilon^{7\cdot 2 \pm 0\cdot 4}. \tag{5.6}$$

The scaling prediction for the exponent is 7·25.

The $\eta \to 0$ behaviour described by (5.4c) cannot be readily studied on the simple cubic lattice. Enting (1974) investigated the corresponding behaviour on the anisotropic FCC lattice and found exponents for G_{010} and G_{001} consistent with scaling predictions.

Along line 3 of figure 1, $T = T_I$, $\eta = 0$ the high-field series gives terms to μ^9. We have obtained the following estimates by evaluating Padé approximants to $1-\mu$ multiplied by the logarithmic derivative of the function in question:

$G_{001} \sim (1-\mu)^{-0\cdot 132 \pm 0\cdot 002}$	scaling predicts	$-0\cdot 13$
$G_{101} \sim (1-\mu)^{0\cdot 5 \pm 0\cdot 1}$	scaling predicts	$0\cdot 4$
$G_{002} \sim (1-\mu)^{0\cdot 83 \pm 0\cdot 05}$	scaling predicts	$0\cdot 8$
$G_{001} \sim (1-\mu)^{0\cdot 90 \pm 0\cdot 05}$	scaling predicts	$0\cdot 86$.

The ratio method did not give any regular exponent estimates. The other technique that was used was that of Gaunt and Sykes (1972) who considered the individual coefficients of the logarithmic derivative since if $f(\mu) \sim (1-\mu)^{-y}$, $\mathrm{d}(\ln f)/\mathrm{d}\mu \sim y/(1-\mu)$ so the individual coefficients tend to y. Coefficients obtained from G_{001} tended to $-0\cdot 132 \pm 0\cdot 002$, coefficients from G_{101} tended to $0\cdot 5 \pm 0\cdot 04$ but showed moderately large oscillations. The coefficients in the other series showed such large oscillations that no exponent estimates could be obtained.

These results add a new class of successful tests of the scaling theory and indicate that the scaling region is sufficiently large for comparatively short series to reveal the scaling behaviour.

6. Investigations of a tricritical point

The anisotropic Ising model with negative interlayer coupling is very similar to real metamagnets such as $FeCl_2$ (Birgeneau *et al* 1974). The distinctive feature of such systems is that as the applied field is increased the continuous transition becomes first order, the point separating these regimes being the tricritical point.

The scaling theory of tricritical points was formulated by Reidel (1972) but we use the formalism of Hankey *et al* (1972).

We assume that the singular part of the free energy can be written as a generalized homogeneous function

$$\lambda G(\epsilon, h, \Delta) = G(\lambda^a \epsilon, \lambda^b h, \lambda^c \Delta). \tag{6.1}$$

The field Δ is the field perpendicular to the coexistence surface and is a staggered field in the Ising metamagnet. ϵ is the deviation from the tricritical point along the direction tangent to the line of critical points. The field h represents deviations from the tricritical point in the $\Delta = 0$ plane but not parallel to the ϵ direction. In figure 1, deviations along either of lines 7 or 8 could be described by h and so each of these paths should exhibit the same tricritical exponents.

Reidel and Wegner (1972) have pointed out that in three dimensions, the tricritical indices should have their mean field values so that $a = \frac{1}{3}$, $b = \frac{2}{3}$, $c = \frac{5}{6}$. There may however also be logarithmic factors included in the tricritical behaviour.

Since we have not included a staggered field in Hamiltonian (2.1) all the exponents that we can study can be expressed in terms of a and b and without a precise estimate of the critical line $T_c(H, -1)$ to define the ϵ direction we can only investigate tricritical exponents involving b.

In particular we expect the following for susceptibility:

$$\chi \sim \begin{cases} (T - T_t)^{-\bar{\gamma}} & H/kT \text{ fixed} \quad (6.2a) \\ (H - H_t)^{-\bar{\gamma}} & T \text{ fixed} \quad (6.2b) \end{cases}$$

and for magnetization:

$$M - M_t \sim \begin{cases} (T - T_t)^{\bar{\beta}} & H/kT \text{ fixed} \quad (6.2c) \\ (H - H_t)^{\bar{\beta}} & T \text{ fixed} \quad (6.2d) \end{cases}$$

where fixed implies fixed at the tricritical point values.

The scaling predictions for exponents are

$$\bar{\gamma} = (2b - 1)/b = \tfrac{1}{2} \tag{6.3a}$$

$$\bar{\beta} = (1 - b)/b = \tfrac{1}{2}. \tag{6.3b}$$

Harbus and Stanley (1972, 1973b) estimated that the tricritical point was located at

$$kT_t/J = 2{\cdot}60 \pm 0{\cdot}05 \tag{6.4a}$$

$$H_t/kT_t = 0{\cdot}72 \pm 0{\cdot}02 \tag{6.4b}$$

or

$$\mu_t = 0{\cdot}237 \pm 0{\cdot}010 \tag{6.4c}$$

$$u_t = 0{\cdot}215 \pm 0{\cdot}006 \tag{6.4d}$$

or

$$x_t = 0{\cdot}381 \pm 0{\cdot}015 \tag{6.4e}$$

$$w_t = 0{\cdot}367 \pm 0{\cdot}007. \tag{6.4f}$$

The investigation of χ along the tricritical isotherm proved unsuccessful. The series is dominated by a singularity at $\mu \approx -0{\cdot}19$. In addition the behaviour for positive real μ

appears to be generally represented by a pole–zero pair and so no sensible exponent estimates could be obtained. This type of behaviour may well indicate significant logarithmic corrections to the simple scaling form (6.2*b*).

We then attempted to estimate the tricritical magnetization M_t. To do this we had to assume the scaling form (6.2*d*) and construct [4, 5] and [5, 4] Padé approximants to $(M-x)^2$ for various values of x. The smallest positive zeros of these approximants were plotted as in figure 2. On the basis of (6.2*d*) the best estimate of M_t should be the value of x for which the zero occurs at μ_t. This leads to

$$M_t = 0{\cdot}70 \pm 0{\cdot}04. \qquad (6.5)$$

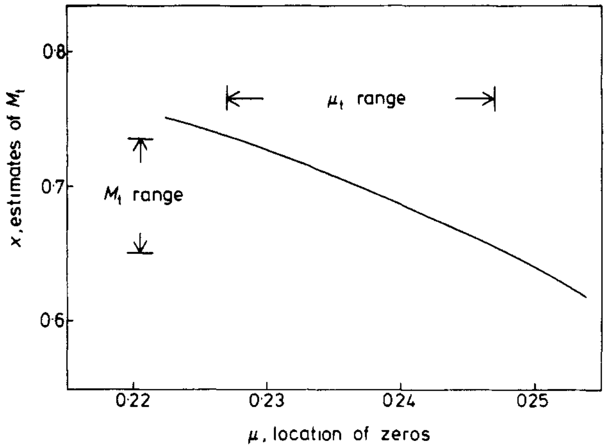

Figure 2. Estimates of the tricritical magnetization, M_t. The graph shows μ, the smallest real zeros of $[M, N]$ Padé approximants to $(M-x)^2$ for $0{\cdot}65 \leq x \leq 0{\cdot}75$. M_t is taken as the average x value for which these lines cut $\mu = \mu_t = 0{\cdot}237$. The full curve is from [4, 5] and [5, 4] approximants.

Since the two approximants give identical μ estimates to with $\frac{1}{4}\%$ it would appear that all the error in M_t arises from uncertainties in μ_t. This is not necessarily true because logarithmic corrections to (6.2*d*) would introduce a systematic bias into the estimates. The value 0·7 is much larger than $M_t = 1/\sqrt{6} = 0{\cdot}408\ldots$ obtained from the mean-field approximation. A large part of this deviation probably results from the fact that the mean-field approximation underestimates H_t (1·35 compared to 1·87) (Bidaux *et al* 1967).

For completeness we also repeated the Harbus and Stanley investigation of χ along the line of H/T fixed using our series with the new term. The results did not, of course, give any major improvement but were generally consistent with the tricritical scaling theory. We content ourselves with giving the exponent estimate $\bar{\gamma} = 0{\cdot}52 \pm 0{\cdot}05$ obtained from Padé approximants to $(0{\cdot}367 - w)\,\mathrm{d}(\ln \chi)/\mathrm{d}w$.

In conclusion it is clear that improvement of our study of the tricritical point requires series including a staggered field so that the strongly divergent staggered susceptibility can be used to locate the transition line. Introducing a staggered field has the additional advantage that low-temperature series can be obtained so that the first-order transition line can be investigated. In addition series for the sublattice (i.e. layer) magnetizations can be obtained. Even though the staggered field is not experimentally variable, its conjugate the layer magnetization is experimentally measurable by means of neutron diffraction (Birgeneau *et al* 1974).

7. An evaluation

The results obtained in the preceding sections are important as a demonstration of the power of high-field series techniques as well as extending studies of the anisotropic Ising model. This is particularly true for loose-packed lattices where the techniques of Sykes *et al* (1965) apply. (For extensions beyond the spin-$\frac{1}{2}$ Ising model see Sykes and Gaunt (1973) and Enting (1975).) Indirect methods such as the partial generating function method and the low–high transformation usually involve large numbers beyond the precision of most computer word-lengths. One solution is to perform all manipulations using one of the many symbolic and algebraic manipulation packages that includes arbitrary precision arithmetic (for a review see Barton and Fitch 1972). Maintaining exact results is important because successive indirect techniques will compound any lack of precision.

During the course of our work a new technique of series analysis has been developed which promises to revolutionize the study of many variable series since it is able to describe crossover between different classes of critical phenomena. The technique was developed by Fisher (1977) and suggests fitting series to a partial differential equation (PDE). This is a generalization of Padé approximants since $P(x)/Q(x) = \mathrm{d}(\ln f(x))/\mathrm{d}x = f'(x)/f(x)$ is equivalent to $P(x)f(x) - Q(x)f'(x) = 0$. The utility of the PDE technique is as yet unknown and so it would be inappropriate to apply it to new situations such as tricritical points. The scaling behaviour around the two-dimensional Ising model is however fairly well understood and the general series could provide a large number of two-variable functions that could be investigated by the new technique. The PDE method does apply to more variables but this would be an undesirable complication in preliminary studies.

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Appendix. Partial generating functions and high-field polynomials

A.1. *Coded expressions for the partial generating functions*

$F_0 = \ln f_0$

$F_1 = (6; 4, 2)$

$F_2 = (11; 8, 2; 0, 0, 1) + 2(11; 6, 4; 1) + 2(10; 4, 4; 2) + 4(10; 6, 2; 0, 2) - 9\frac{1}{2}(12; 8, 4)$

$$
\begin{aligned}
F_3 = {} & 8(13;6,3;1,2,0;0,1)+16(14;6,4;2,2)+12(14;8,2;0,4)+2(14;4,6;4)\\
& +8(15;6,6;3)+24(15;8,4;1,2)+8(15;8,4;2,0,1)\\
& +8(15;10,2;0,2,1)-50(16;8,6;2)+8(16;10,4;1,0,1)\\
& -112(16;10,4;0,2)+1(16;12,2;0,0,2)-64(17;10,6;1)\\
& -32(17;12,4;0,0,1)+151\tfrac{1}{3}(18;12,6)+4(14;5,6;2,0,0;1)\\
& +4(14;8,3;0,2,0;0,1)+4(14;9,2;0,2,0;0,0,1)\\
F_4 = {} & 8(16;6,4;2,3,0;0,0,0,0;0,1)+4(16;8,2;1,4,0;0,0,0,0;0,0,1)\\
& +2(16;8,4;0,0,0;0,4)+4(16;8,2;0,4,0;0,2)\\
& +8(16;6,4;2,2,0;0,2)+1(17;4,8;4,0,0;0,0,0,0;1)\\
& +2(17;10,2;0,4,0;0,0,0,0;0,0,1)+24(17;6,5;3,2,0;0,1)\\
& +48(17;8,3;1,4,0;0,1)+16(17;7,5;1,2,0;1,1)\\
& +16(17;8,4;1,2,0;0,2)+16(17;9,3;1,2,0;0,1,1)\\
& +2(18;4,8;6)+32(18;6,6;4,2)+92(18;8,4;2,4)\\
& +36(18;10,2;0,6)+8(18;5,8;4,0,0;1)+40(18;7,6,2,2,0;1)\\
& +64(18;8,5;2,2,0;0,1)+24(18;9,4;2,2,0;0,0,1)\\
& +32(18;10,3;0,4,0;0,1)+24(18;10,3;1,2,1;0,1)\\
& +24(18;11,2;0,4,0;0,0,1)+8(18;6,8;2,0,0;2)\\
& +4(18;10,4;0,2,0;0,2)+8(18;11,3;0,2,0;0,1,1)\\
& +4(18;12,2;0,2,0;0,0,2)+2(18;8,4;4,0,2)\\
& +16(19;6,8;5)+144(19;8,6;3,2)+24(19;8,6;4,0,1)\\
& +160(19;10,4;1,4)+96(19;10,4;2,2,1)+40(19;12,2;0,4,1)\\
& +20(19;7,8;3,0,0,1)+24(19;9,6;2,0,1;1)\\
& -240(19;10,5;1,2,0;0,1)+36(19;11,4;1,2,0;0,0,1)\\
& +12(19;12,3;0,2,1;0,1)+8(19;13,2;0,2,1;0,0,1)\\
& -116(20;8,8;4)-788(20;10,6;2,2)\\
& +80(20;10,6;3,0,1)+128(20;12,4;1,2,1)+18(20;12,4;2,0,2)\\
& -762(20;12,4;0,4)+12(20;14,2;0,2,2)\\
& -148(20;9,8;2,0,0;1)-148(20;13,4;0,2,0;0,0,1)\\
& -148(20;12,5;0,2,0;0,1)-494(21;10,8;3)\\
& -1336(21;12,6;1,2)-364(21;12,6;2,0,1)\\
& -512(21;14,4;0,2,1)+16(21;14,4;1,0,2)\\
& +1(21;16,2;0,0,3)+1202(22;12,8;2)\\
& +3132(22;14,6;0,2)-458(22;14,6;1,0,1)
\end{aligned}
$$

$$-67\tfrac{1}{2}(22; 16, 4; 0, 0, 2) + 1910(23; 14, 8; 1)$$
$$+955(23; 16, 6; 0, 0, 1) - 3005{\cdot}75(24; 16, 8)$$

A.2. Anisotropic Ising model high-field polynomials

$$L_1 = +1u^2v$$

$$L_2 = -3\tfrac{1}{2}u^4v^2 + 1u^4v + 2u^3v^2$$

$$L_3 = +21\tfrac{1}{3}u^6v^3 - 12u^6v^2 + 1u^6v - 24u^5v^3 + 8u^5v^2 + 6u^4v^3$$

$$L_4 = -162\tfrac{3}{4}u^8v^4 + 135u^8v^3 - 25\tfrac{1}{2}u^8v^2 + 1u^8v + 270u^7v^4 - 168u^7v^3 + 16u^7v^2 - 135u^6v^4 + 48u^6v^3 + 2u^6v^2 + 18u^5v^4 + 1u^4v^4$$

$$L_5 = +1u^{10}v + 1406\tfrac{1}{5}u^{10}v^5 - 1536u^{10}v^4 + 468u^{10}v^3 - 44u^{10}v^2 - 3072u^9v^5 + 2752u^9v^4 - 576u^9v^3 + 24u^9v^2 + 2312u^8v^5 - 1520u^8v^4 + 126u^8v^3 - 664u^7v^5 + 240u^7v^4 + 24u^7v^3 + 35u^6v^5 + 8u^6v^4 + 8u^5v^5 + 8u^8v^2$$

$$L_6 = -13150\tfrac{2}{3}u^{12}v^6 + 17790u^{12}v^5 - 7566u^{12}v^4 + 1203\tfrac{1}{3}u^{12}v^3 - 67\tfrac{1}{2}u^{12}v^2 + 1u^{12}v + 35580u^{11}v^6 - 41360u^{11}v^5 + 13660u^{11}v^4 - 1392u^{11}v^3 + 32u^{11}v^2 - 35812u^{10}v^6 + 33644u^{10}v^5 - 7124u^{10}v^4 + 132u^{10}v^3 + 16u^{10}v^2 + 16066\tfrac{2}{3}u^9v^6 - 10832u^9v^5 + 612u^9v^4 + 144u^9v^3 + 2u^9v^2 - 2729u^8v^6 + 872u^8v^5 + 200u^8v^4 + 6u^8v^3 - 74u^7v^6 + 96u^7v^5 + 8u^7v^4 + 40u^6v^6 + 2u^5v^6$$

$$L_7 = +129919\tfrac{1}{7}u^{14}v^7 - 209412u^{14}v^6 + 114845u^{14}v^5 - 26440u^{14}v^4 + 2580u^{14}v^3 - 96u^{14}v^2 + 1u^{14}v - 418824u^{13}v^7 + 597000u^{13}v^6 - 271168u^{13}v^5 + 46384u^{13}v^4 - 2760u^{13}v^3 + 40u^{13}v^2 + 528190u^{12}v^7 - 640248u^{12}v^6 + 218576u^{12}v^5 - 20504u^{12}v^4 - 84u^{12}v^3 + 24u^{12}v^2 - 324048u^{11}v^7 + 312912u^{11}v^6 - 63272u^{11}v^5 - 1600u^{11}v^4 + 360u^{11}v^3 + 8u^{11}v^2 + 94200u^{10}v^7 - 62724u^{10}v^6 + 625u^{10}v^5 + 1424u^{10}v^4 + 84u^{10}v^3 - 8024u^9v^7 + 960u^9v^6 + 1272u^9v^5 + 128u^9v^4 - 1302u^8v^7 + 696u^8v^6 + 112u^8v^5 + 8u^8v^4 + 112u^7v^7 + 24u^7v^6 + 22u^6v^7$$

$$L_8 = -1336290\tfrac{3}{8}u^{16}v^8 + 2498929u^{16}v^7 - 1681690\tfrac{2}{4}u^{16}v^6 + 513297u^{16}v^5 - 74247\tfrac{3}{4}u^{16}v^4 + 4893u^{16}v^3 - 129\tfrac{2}{4}u^{16}v^2 + 1u^{16}v + 4997858u^{15}v^8 - 8427736u^{15}v^7 + 4884924u^{15}v^6 - 1197624u^{15}v^5 + 124394u^{15}v^4 - 4824u^{15}v^3 + 48u^{15}v^2 - 7577249u^{14}v^8 + 11212196u^{14}v^7 - 5280832u^{14}v^6 + 904496u^{14}v^5 - 43074u^{14}v^4 - 660u^{14}v^3 + 32u^{14}v^2 + 5911518u^{13}v^8 - 7364680u^{13}v^7 + 2519472u^{13}v^6 - 185808u^{13}v^5 - 13376u^{13}v^4 + 528u^{13}v^3 + 16u^{13}v^2 - 2444771\tfrac{2}{4}u^{12}v^8 + 2380142u^{12}v^7 - 429606u^{12}v^6 - 41696u^{12}v^5 + 3379u^{12}v^4 + 354u^{12}v^3 + 2u^{12}v^2$$

$$+459372u^{11}v^{8}-281336u^{11}v^{7}-23956u^{11}v^{6}+9304u^{11}v^{5}$$
$$+1382u^{11}v^{4}+24u^{11}v^{3}-2805u^{10}v^{8}-18088u^{10}v^{7}+6120u^{10}v^{6}$$
$$+1352u^{10}v^{5}+98u^{10}v^{4}-8386u^{9}v^{8}+3224u^{9}v^{7}+1032u^{9}v^{6}+144u^{9}v^{5}$$
$$-190\tfrac{2}{4}u^{8}v^{8}+352u^{8}v^{7}+32u^{8}v^{6}+1u^{8}v^{4}+134u^{7}v^{8}+6u^{6}v^{8}$$

$$L_9=+14175534\tfrac{1}{9}u^{18}v^{9}-30160276u^{18}v^{8}+24079426u^{18}v^{7}-9215812u^{18}v^{6}$$
$$+1802383u^{18}v^{5}-178972u^{18}v^{4}+8493\tfrac{1}{3}u^{18}v^{3}-168u^{18}v^{2}+1u^{18}v$$
$$-60320552u^{17}v^{9}+117370888u^{17}v^{8}-82843064u^{17}v^{7}$$
$$+26700656u^{17}v^{6}-4091356u^{17}v^{5}+284144u^{17}v^{4}-7728u^{17}v^{3}$$
$$+56u^{17}v^{2}+106844296u^{16}v^{9}-186353272u^{16}v^{8}+111878056u^{16}v^{7}$$
$$-28048840u^{16}v^{6}+2792832u^{16}v^{5}-71336u^{16}v^{4}-1734u^{16}v^{3}$$
$$+40u^{16}v^{2}-101274688u^{15}v^{9}+153869616u^{15}v^{8}-73638240u^{15}v^{7}$$
$$+11973466\tfrac{2}{3}u^{15}v^{6}-254520u^{15}v^{5}-43792u^{15}v^{4}+480u^{15}v^{3}$$
$$+24u^{15}v^{2}+54452210u^{14}v^{9}-68846316u^{14}v^{8}+22951672u^{14}v^{7}$$
$$-964884u^{14}v^{6}-263081u^{14}v^{5}-380u^{14}v^{4}+804u^{14}v^{3}+8u^{14}v^{2}$$
$$-15714036u^{13}v^{9}+15039376u^{13}v^{8}-2111432u^{13}v^{7}-511664u^{13}v^{6}$$
$$+8996u^{13}v^{5}+6240u^{13}v^{4}+192u^{13}v^{3}+1703080u^{12}v^{9}-742880u^{12}v^{8}$$
$$-318948u^{12}v^{7}+36872u^{12}v^{6}+12644u^{12}v^{5}+960u^{12}v^{4}+6u^{12}v^{3}$$
$$+174648u^{11}v^{9}-196368u^{11}v^{8}+14872u^{11}v^{7}+9832u^{11}v^{6}+2080u^{11}v^{5}$$
$$+48u^{11}v^{4}-33424u^{10}v^{9}+4808u^{10}v^{8}+7174u^{10}v^{7}+1632u^{10}v^{6}$$
$$+16u^{10}v^{5}+8u^{10}v^{4}-4884u^{9}v^{9}+2888u^{9}v^{8}+504u^{9}v^{7}$$
$$+56u^{9}v^{6}+16u^{9}v^{5}+444u^{8}v^{9}+96u^{8}v^{8}+72u^{7}v^{9}+1u^{6}v^{9}.$$

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