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LETTER TO THE EDITOR

Mean-field renormalisation group transformations for the triangular Ising antiferromagnet

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Abstract. The mean-field renormalisation group of Indekeu *et al* is applied to the antiferromagnetic nearest-neighbour Ising model on the triangular lattice. The resulting phase diagram in the temperature–field plane is in good agreement with other calculations, while the predicted specific-heat index, α, is negative and thus qualitatively wrong. The study indicates that the method may be a useful approach, at least for determining phase diagrams, for frustrated systems and systems with competing interactions where conventional mean-field theory is dubious.

Recently a new real-space renormalisation group method for calculating critical properties of lattice systems has been proposed (Indekeu *et al* 1982). This method, which in the following will be called the 'mean-field renormalisation group' (MFRG), has been applied to a diversity of systems, including classical and quantum spins (Indekeu *et al* 1982), random systems including spin glass (Droz *et al* 1982) and geometric phase transitions (De'Bell 1983), and seems to improve substantially on mean-field (MF) calculations of equal complexity. The motivation for the work reported in this letter is to shed light on the applicability of MFRG to systems with competing interactions and frustration. This is an open question since MFRG in part is based on a MF line of thought and it is well known that MF theory often fails in systems with frustration of competing interactions (Burley 1965, Binder and Landau 1980). The MF concept, which contains most of the physics in the ferromagnetic case, seems somehow to imply a neglect of frustration effects. One might therefore suspect that MFRG, like MF theory, is dubious when investigating frustrated systems. MFRG makes, on the other hand, use of the MF concept at a different level than does conventional MF-theory. Both MF and MFRG consider the behaviour of finite clusters in a mean field (symmetry breaking boundary conditions), but while MF theory identifies the order parameter of this field with the order parameter of the cluster, MFRG only assumes that the order parameter *scales* in the same way.

The model considered in this letter is the antiferromagnetic nearest-neighbour Ising model on the triangular lattice. The Hamiltonian is

$$-\beta\mathscr{H} = K\left(h\sum_{i}\sigma_i - \sum_{\langle i,j\rangle}\sigma_i\sigma_j\right) \qquad (1)$$

where β is the inverse temperature, $K>0$, the nearest-neighbour coupling in units of temperature, h is an external magnetic field and the sums run over all spins and all nearest-neighbour pairs, respectively. Due to symmetry only non-negative h need to be considered. In zero field this model is fully frustrated with an infinitely degenerate ground state, while the ground state is threefold degenerate, with two sublattice magnetisations +1 and one −1; in non-zero field $h<6$. The ordered phase can be characterised by a two-component order parameter which measures differences between the three sublattice magnetisations; we use

$$O=(o_1,o_2)=(\tfrac{1}{4}(m_1+m_2-2m_1),\tfrac{1}{4}(m_1-2m_2+m_3)) \tag{2}$$

where m_n is the nth sublattice magnetisation. The fully frustrated zero-field case is exactly solvable (Houtappel 1950) and shows no phase transition at non-zero temperature. This exact feature is not reproduced by MF-type approaches (Kasteleijn 1956, Burley 1965, Campbell and Schick 1972). The critical exponents in non-zero fields should, following universality and symmetry arguments, be identical to those of the exactly solved hard-hexagon model (Baxter 1980) and the three-state Potts model (Alexander 1975, den Nijs 1979, Nienhuis *et al* 1980a, b, Schick 1981). In particular the thermal exponent is $y_t=\frac{6}{5}$ giving a specific heat index $\alpha=\frac{1}{3}$†. The critical line in the h, K plane is by now quite well known through calculations by diverse methods (Metcalf 1973, Schick *et al* 1977, Kinzel and Schick 1981, Dóczi-Réger and Hemmer 1981). The derivative of the critical line at $h_c=6$ ($T=0$) is known exactly (Baxter 1980):

$$(\mathrm{d}(1/K_c)/\mathrm{d}h)_{h=6}=-\tfrac{1}{2}\ln(11/2+5\sqrt{5}/2) \tag{3}$$

while the derivative at $h_c=0$ ($T=0$) from scaling arguments is expected to be infinite (Kinzel and Schick 1981).

To sum up: the present model is a simple well studied system with frustration, where MF theory fails to produce a qualitatively correct phase diagram. Application of MFRG to this model should therefore give valuable indications about the performance of this method in systems with competing interactions and frustration in general.

MFRG is based upon comparison of the behaviour of clusters of different size in the presence of a mean field at the boundary. As already mentioned it is convenient in the present case to replace the sublattice magnetisations, m_1, m_2 and m_3, by the order parameter $O=(o_1,o_2)$ (1), and the mean magnetisation, $m=\frac{1}{3}(m_1+m_2+m_3)$. The corresponding three magnetisation parameters of the surrounding mean field are denoted by $\Omega=(\omega_1,\omega_2)$ and μ. Calculation of the order parameters and mean magnetisation to the lowest order in Ω, for a cluster of N spins, gives equations of the form

$$m=M(h,\mu,K), \qquad O=A(h,\mu,K)\Omega. \tag{4}$$

Doing the same for a cluster of a smaller size N' gives similarly

$$m'=M'(h',\mu',K'), \qquad O'=A'(h',\mu',K')\Omega'. \tag{5}$$

One then assumes finite-size scaling (Fisher 1971, Suzuki 1977) which is expected to be exact when $N, N'\to\infty$ and K and K' are close to K_c.

$$h'=h, \tag{6}$$

$$O'(h',\mu',K')=(N/N')^{-\beta/d\nu}O(h,\mu,K), \tag{7}$$

$$K'=(N/N')^{1/d\nu}K-[(N/N')^{1/d\nu}-1]K_c, \tag{8}$$

† The zero-field model has a phase transition at $T=0$, and it should be noted that this belongs to a different universality class having a thermal exponent $y_t=0$ (Domany *et al* 1978, Alexander and Pincus 1980).

where β and ν are the order parameter and correlation length critical indices, respectively, d the dimensionality of the system and K_c the bulk critical coupling (inverse critical temperature). Expanding (7) to the lowest order in Ω and Ω', (4) and (5), and assuming that Ω scales in the same way as O (7) gives

$$A'(h, \mu', K') = A(h, \mu, K). \tag{9}$$

The mean magnetisation, and hence μ, has its own size dependence which is not governed by finite-size scaling. It is natural to approximate this size dependence by the MF ansatz $m = \mu$ and $m' = \mu'$. Equations (4), (5) and (9) thus reduce to the following system of equations which, via elimination of μ and μ', represent an approximate renormalisation group transformation, $K' = K'(K)$:

$$\mu = M(h, \mu, K), \qquad \mu' = M'(h, \mu', K'), \qquad A'(h, \mu', K') = A(h, \mu, K). \tag{10}$$

Equation (8) shows that the fixed point of this transformation, $K^* = K' = K$, can be identified as the critical coupling, K_c, in the external magnetic field h.

One may expect the finite-size scaling law (6)–(8) to be approximately valid only when the differences in the shape and size of the two clusters in question can be eliminated by simply adjusting the length scales in one or both space directions. For the present model this, and the requirement that all sublattices should be equivalent in the cluster, which was implicitly assumed when deriving (4), limits the choice of clusters substantially. For clusters of size $N < 20$ only three triangular clusters, with 3, 6 and 15 spins respectively, come into consideration; these are shown in figure 1.

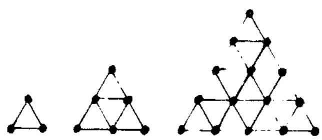

Figure 1. The three clusters used in the calculation.

For the three-spin cluster the explicit expressions in (4) are easily evaluated, giving

$$m = \frac{\sinh(3\alpha) + \exp(4K)\sinh(\alpha)}{\cosh(3\alpha) + 3\exp(4K)\cosh(\alpha)}, \qquad O = \frac{8K\exp(4K)\cosh(\alpha)}{\cosh(3\alpha) + 3\exp(4K)\cosh(\alpha)}\Omega, \tag{11}$$

with

$$\alpha = (h - 4\mu)K,$$

while the corresponding expressions for the 6- and 15-spin clusters are too complicated to be reproduced here. Simple MF theory, i.e. putting $m = \mu$ and $O = \Omega$ and solving (4), gives a zero-field critical temperature of 2.50, 2.20 and 1.84 for the 3-, 6- and 15-spin clusters, respectively, in contrast to the exact value of zero. Applying the MFRG to the same clusters (10) leads to the phase diagrams, for the (3, 6) and (6, 15) approximations, shown in figure 2. Except for a rather pathological low-temperature part the (6, 15) approximation gives a critical line in reasonable agreement with other calculations.

One would like to know why the method is deficient at low temperatures. An indication of this may be given by noting that the function A in (4) is nothing but a

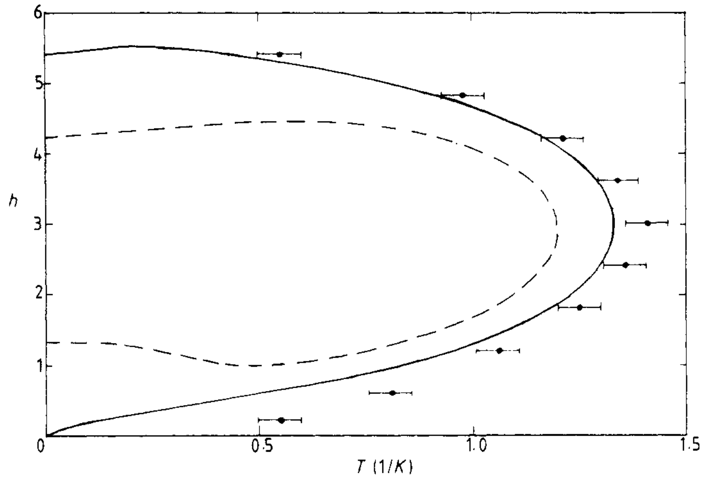

Figure 2. Phase diagram in the temperature–magnetic-field plane. The broken line is the (3, 6) approximation, the full line the (6, 15) approximation, and the points are MC results (Metcalf 1973).

sum over selected correlations in the cluster. For very low temperatures these correlations are almost unity, and from this trivial value no information on couplings can be deduced. With increasing cluster size the temperature range for which the correlations are almost trivial decreases slowly (logarithmically).

The correlation-length index, ν, can be found by linearising the transformation (10) about the fixed point

$$\Delta K' = \lambda \Delta K, \tag{12}$$

and noting that (8) gives

$$\lambda = (N/N')^{1/d\nu}. \tag{13}$$

The thermal exponent, y_t, can then be found from the well known relation $y_t = 1/\nu$ (Stanley 1971). This procedure will give a different exponent for each value of the magnetic field as shown in figure 3. As a consequence of universality one expects a unique exponent, and within phenomenological scaling, which is very close in spirit to the present method and shares the same weak point, much effort has been put into developing methods for calculation of exponents and for singling out the best value of the exponent (Kinzel and Schick 1981, Burkhardt and van Leeuwen 1982). These methods may be applied in MFRG too, but for the present purpose it suffices to note that the exponent has plateau values of $y_t \approx 0.7$ and $y_t \approx 0.86$ in the (3, 6) and (6, 15) approximation, respectively, while the correct value is $y_{t,\text{exact}} = 1.2$. The calculated thermal exponent is thus very poor, and it implies a *negative* specific heat index, which is qualitatively wrong†. The capability of the method to predict exponents is poor in the ferromagnetic case too (Indekeu *et al* 1982), but one expects the exponents to converge towards the exact values for larger clusters.

The present study indicates that the mean field renormalisation group may be a useful approach for systems with competing interactions and frustration, at least as

† This is a property this method shares with a more conventional real space RG (Schick *et al* 1977).

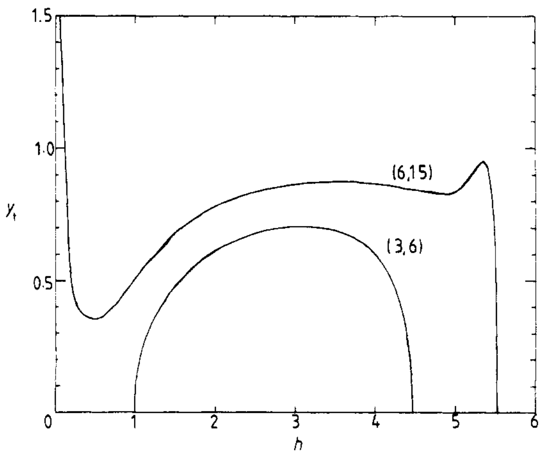

Figure 3. Thermal exponent as a function of magnetic field for the (3, 6) and (6, 15) approximations, respectively. The correct value of the exponent is 1.2 in all fields $0 < h \leq 6$.

far as determination of critical temperatures is concerned. The method is unreliable for low temperature phase transitions though, and this should call for caution when applying it to low temperature problems such as spin glasses (Droz *et al* 1982).

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