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Mean-field renormalisation group approach for the axial next-nearest-neighbour Ising model

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Abstract. The critical properties of the axial next-nearest-neighbour Ising (ANNNI) model are investigated by using the mean-field renormalisation group approach. Linear and double chain clusters lying along the axial direction are considered. Phase diagrams for the model in two and three dimensions and estimates of thermal exponents are obtained.

1. Introduction

In recent years, considerable attention has been focused on the study of the axial next-nearest-neighbour Ising (ANNNI) model. Despite being perhaps one of the simplest extensions of the Ising model with competing interactions, it displays a very rich critical behaviour. The corresponding Hamiltonian model, with isotropic ferromagnetic nearest-neighbour interactions $J_1 > 0$, can be defined as

$$H = -\tfrac{1}{2} \sum_{i,j,k} (J_1 S_{i,j,k} S_{i\pm1,j\pm1,k\pm1} - J_2 S_{i,j,k} S_{i\pm2,j,k}) \qquad S_{i,j,k} = \pm 1 \qquad (1)$$

where $J_2 > 0$ is a competing antiferromagnetic interaction between next-nearest-neighbour spins along the i direction. In one dimension, model (1) was exactly solved by Stephenson (1970). In higher dimensions, it has been shown that the system exhibits paramagnetic, ferromagnetic and modulated phases, as well as a Lifshitz point on the ferromagnetic side at non-zero temperature for the three-dimensional model.

In three dimensions, the high-temperature region of the phase diagram and the vicinity of the Lifshitz point (LP) have been investigated by renormalisation group methods (Hornreich *et al* 1975, Hornreich 1980), high-temperature series expansions (Redner and Stanley 1977, Oitmaa 1985) and Monte Carlo simulations (Selke 1978). The LP has been located at an absolute temperature $T \neq 0$. In the low-temperature region, the model has been studied by low-temperature series expansions (Fisher and Selke 1980), Monte Carlo simulations (Selke and Fisher 1979), effective pair, triplet, etc, wall-wall interactions (Szpilka and Fisher 1986) and various mean-field theories (Bak and von Boem 1980, Yokoi *et al* 1981, Bak 1982, Selke and Duxbury 1984). It has been shown that the ground state of the model is ferromagnetic for $2J_2 < J_1$, and for $2J_2 > J_1$ it exhibits a periodically extended sequence of two-up and two-down ferromagnetic planes of spins lying along the i direction. The point $T = 0$, $2J_2 = J_1$ is a multiphase point with an infinite ground-state degeneracy.

In two dimensions, the calculations performed on the ANNNI model include Monte Carlo simulations (Selke and Fisher 1980) and high-temperature expansions (Rujan

1981), which localise a LP on the ferromagnetic side of the phase diagram at a non-zero temperature. According to the current consensus, however, a disordered phase is stable down to $T=0$ with no LP at finite temperature for $J_2/J_1<0.5$. This point of view is supported, among other works, by exact solutions (on a special line) of an equivalent Hamiltonian (Peschel and Emery 1981), free fermion approximations (Villain and Bak 1981), Monte Carlo simulations with a careful finite-size analysis (Selke 1981) and a finite-size scaling treatment (Beale *et al* 1985). More recently, a calculation within the framework of the cluster variation method (Finel and de Fontaine 1986) indicated the absence of a LP at a finite temperature for $J_2/J_1<0.5$.

In the present work, we have studied the ANNNI model as given by the Hamiltonian (1) within the mean-field renormalisation group (MFRG) framework (Indekeu *et al* 1982). According to this approach, the magnetisations per spin for two distinct clusters surrounded by symmetry breaking fields are compared assuming these fields scale in the same way as the magnetisations themselves. This method allows one to obtain a recursion relation among the parameters of the system and thereby the critical points of the model. In addition, it allows one to obtain estimates for thermal exponents by means of a standard procedure. The clusters we have considered are the linear chain (cluster I) and the double chain (cluster II) as indicated in figure 1. The expressions of the magnetisations for both cases are trivially connected to their respective susceptibilities which, in the present case, can be evaluated through a simple extension of the transfer matrix procedure used for calculating spin correlation functions of the Ising model on the linear chain (Marsh 1966).

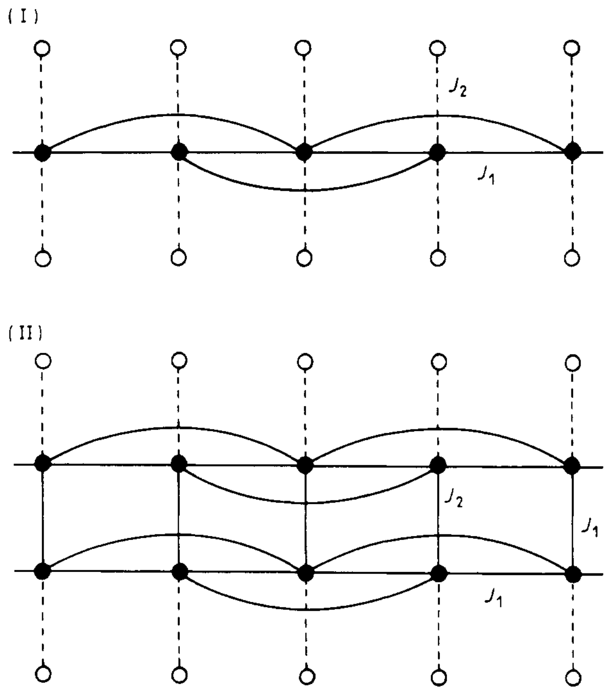

Figure 1. Schematic representation of the linear chain cluster (I) and the double chain cluster (II) in two dimensions. The nearest-neighbour couplings are ferromagnetic and the next-nearest-neighbour couplings are antiferromagnetic. The surrounding spins in each cluster are represented by open circles.

This paper is organised as follows. We first compute the magnetisations per spin for clusters I and II and present the corresponding mean-field results. The phase diagram obtained from the MFRG method is discussed in § 3, and we close the paper with some final comments in § 4.

2. Magnetisations and mean-field approximations

The first step of our calculation consists in obtaining the magnetisation per spin m_L of the cluster I in the presence of a local field h_i' acting on each spin S_i of the linear chain. As required by the MFRG method (Indekeu *et al* 1982), these local fields are given by

$$h_i' = (z-2)J_1 b_i' \tag{2}$$

where $z = 2d$ is the lattice coordination number and b_i' denote the fixed magnetisations of the surrounding spins of cluster I. As $b_i' \ll 1$, and consequently $h_i' \ll 1$, one can use the linear response theory to obtain

$$m_L(K_1', K_2', q') = \chi_L(K_1', K_2', q')(z-2)K_1' b_{q'}' \tag{3}$$

where $K_1' = \beta J_1$ and $K_2' = \beta J_2$ with $\beta = 1/k_B T$ and q' is the wavevector along the axial direction. $\chi_L(K_1', K_2', q')$ is the q'-dependent susceptibility per spin of the linear chain. At this point, some information about the criticality of the $(d>1)$-dimensional model can be extracted via mean-field methods. The q'-dependent susceptibility in the paramagnetic phase for the $d>1$ system can be written as (Scalapino *et al* 1975)

$$\chi_d(K_1', K_2', q') = \frac{\chi_L(K_1', K_2', q')}{1-\chi_L(K_1', K_2', q')(z-2)K_1'} \qquad d>1. \tag{4}$$

The transition temperature and the corresponding periodicity wavenumber are then obtained by the values for which the susceptibility (4) first diverges as the temperature is lowered. In this sense, the interactions along the axial direction are exactly taken into account while the perpendicular interactions are treated in a mean-field way. Such an analysis has been previously done by Pires *et al* (1982). In their work, the linear chain susceptibility was calculated by using the exact results for the correlation functions obtained by Stephenson (1970). They have shown that the results obtained from (4) improve considerably on those of the usual mean-field theories. This approach, however, can just pick up the second-order transition line from the paramagnetic-ferromagnetic phases and paramagnetic-modulated phases. No information about the low-temperature modulated phases can be obtained from equation (4).

The next step consists in obtaining the magnetisation per spin for cluster II. The local field acting on each pair of spins of the double chain is now given by

$$h_i = (z-3)J_1 b_i \tag{5}$$

where b_i are the fixed magnetisations of the surrounding spins of cluster II. For $b_i \ll 1$ one can write

$$m_D(K_1, K_2, q) = \chi_D(K_1, K_2, q)(z-3)K_1 b_q \tag{6}$$

where the quantities appearing in (6) are analogous to those defined for cluster I. The calculation of the q-dependent double chain susceptibility $\chi_D(K_1, K_2, q)$ follows from an extension of Marsh's prescription (March 1966) for evaluating spin correlation functions. One first defines four appropriate 16×16 diagonal 'spin matrices' related to the double chain transfer matrix, quite analogous to the 2×2 spin matrix of the Ising linear chain of spins. The procedure is then essentially the same as that used for calculating spin-pair correlation functions through a product of matrices. Although straightforward, the results are rather too lengthy to reproduce here.

At this stage, it is worth performing a mean-field calculation similar to that done previously for cluster I. The q-dependent susceptibility in the paramagnetic phase is now given by

$$\chi_d(K_1, K_2, q) = \frac{\chi_D(K_1, K_2, q)}{1-\chi_D(K_1, K_2, q)(z-3)K_1} \qquad d>1. \tag{7}$$

As before, the critical temperature and the critical axial wavevector are determined by the values for which the denominator of (7) vanishes (Pires *et al* 1982). The critical line separating the paramagnetic phase as a function of the ratio J_2/J_1 obtained from the present double chain (mean-field) approximation (referred to as DCA) is shown in figure 2 together with those previously obtained by the linear chain (mean-field) approximation (Pires *et al* 1982) (referred to as LCA) and the usual mean-field (MF) approximation for the three-dimensional model. A noticeable improvement is achieved by increasing the width of the clusters. The critical axial wavevector q_c, as a function of J_2/J_1, along the paramagnetic-modulated transition line is zero (at the LP) and approaches the value $\pi/2$ (as $J_2/J_1 \to \infty$) for all approximations. The location of the LP, however, is almost coincident with the MF ratio $J_2/J_1 = 0.25$. Again, no information about the modulated low-temperature region of the phase diagram can be obtained from equation (7). Moreover, all critical exponents remain exactly the same as those of the usual MF theory.

In two dimensions, similar results to those shown in figure 2 are obtained in LCA and DCA approximations. The critical behaviour thus obtained for the ANNNI model in both two and three dimensions is a signature of the mean-field character of the

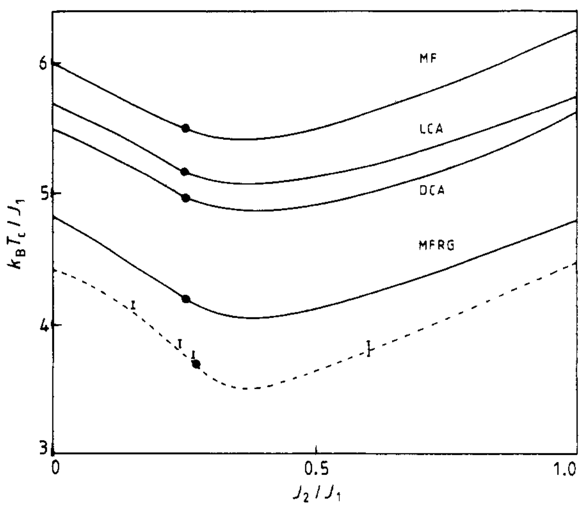

Figure 2. Paramagnetic critical line for the three-dimensional model as a function of J_2/J_1 according to several approximations. The dots on the curves represent the Lifshitz point. The results of a Monte Carlo simulation are represented by the error bars and of high-temperature series expansions by the broken curve.

approximations employed, which do not distinguish, in a qualitative way, the dimensionality of the system for $d > 1$.

3. Mean-field renormalisation group approach

The magnetisations m_L and m_D of the previous section can be combined under renormalisation group ideas by imposing a scaling relation of the form $m_L = \xi m_D$ and assuming a similar scaling relation between b'_q and b_q, i.e. $b'_{q'} = \xi b_q$, yielding

$$(z-2)K'_1\chi_L(K'_1, K'_2, q') = (z-3)K_1\chi_D(K_1, K_2, q) \tag{8}$$

which is independent of the scaling factor ξ. Equation (8) is viewed as a renormalisation recursion relation among the parameters K'_1, K'_2, q' and K_1, K_2, q. It is clear that one cannot determine the complete renormalisation flow diagram in the parameter space of the Hamiltonian (1) from this equation alone. In fact, this is a general trend of the MFRG when the Hamiltonian under study has more than one parameter. However, as has been done in the study of other lattice spin systems (Droz *et al* 1982, Plascak 1984), one can look first at the fixed-point solutions associated with equation (8), namely

$$(z-2)\chi_L(K_1, K_2, q) = (z-3)\chi_D(K_1, K_2, q). \tag{9}$$

From the above relation one can obtain the critical surface of model (1) by computing $(K_1^c)^{-1} = k_B T_c/J_1$ as a function of the ratio J_2/J_1 related to each mode q. For the three-dimensional model, we can obtain with equation (9) a paramagnetic critical line which is shown in figure 2 together with the previous mean-field results as well as those of high-temperature series expansions (Oitmaa 1985) and a Monte Carlo coarse-graining calculation (Kaski and Selke 1985) for comparison. One notices a good agreement of the present MFRG result on this phase boundary with the curves given by more accurate methods. The LP is located at the ratio $J_2/J_1 = 0.255$ which should be compared to the value $J_2/J_1 = 0.265$ obtained through the Monte Carlo calculation and to $J_2/J_1 = 0.27$ obtained by high-temperature series expansions. It should be stressed that the present choice of clusters does not allow one to capture low-temperature features of the phase diagram, since none of them carry the cubic symmetry of the lattice.

On the other hand, for the two-dimensional model, we have obtained through equation (9) the phase diagram shown in figure 3, which displays some curves for $q \neq 0$ in the low-temperature region. This result is certainly correlated to the two-dimensional character of cluster II. Although a detailed description of the phase diagram cannot be obtained by the present approach, the lines separating the modulated phases for $q = \pi/2$ and $q = 0$ are within the limits given by the finite-size scaling procedure of Beale *et al* (1985), which also employs infinite strips with finite widths. Nevertheless, it is not surprising that in the present treatment a LP at a non-zero temperature on the ferromagnetic side is obtained, as in previous mean-field calculations, since the MFRG still carries a mean-field character, which is absent in the phenomenological finite-size scaling procedure employed by Beale *et al* (1985). Furthermore, critical thermal exponents for the two-dimensional case can be estimated from equation (8) by computing

$$|dK'_1/dK_1|_{FP} = l^{1/\nu_T} \tag{10}$$

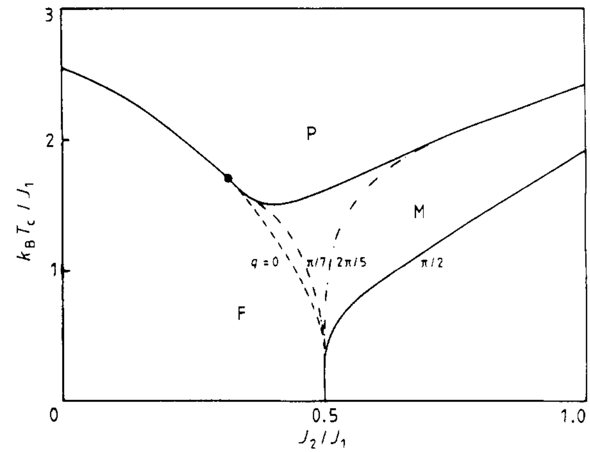

Figure 3. Phase diagram of the two-dimensional model obtained through the MFRG. The dot represents the Lifshitz point (artificially generated by the method). P is the paramagnetic phase, F the ferromagnetic phase and M the modulated phase.

where the derivative is taken at the fixed points given by equation (9), and $l=2$ is the rescaling factor related to the present clusters for the two-dimensional model (Plascak and Silva 1986). The critical exponents ν_T are displayed in figure 4. Although a noticeable crossover is observed at the multiphase point $J_2/J_1=0.5$ for the line $q=\pi/2$, one can also observe a pathological behaviour of ν_T along the paramagnetic line. This behaviour is intrinsically related to the mean-field character of the method which, as has been mentioned above, is more accurate in three dimensions. A calculation of the thermal exponent would further require the knowledge of the scaling factor l which is by no means obvious in this case. However, by merely evaluating the derivative in equation (10) at the fixed points it is possible to get some evidence of a crossover near the LP which is in agreement with the results of Kaski and Selke (1985).

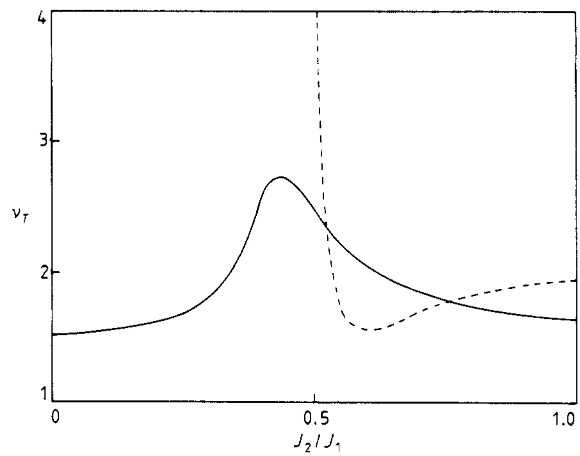

Figure 4. Critical thermal exponent as a function of the ratio J_2/J_1 for the two-dimensional model. The full curve refers to the paramagnetic line (quite probably an artefact of the method). The broken curve refers to $q=\pi/2$ (see figure 3).

4. Final comments

Although the present approach does not yield the expected phase diagram for the two-dimensional ANNNI model, especially its low-temperature complex behaviour for $d > 1$, it has been shown to be a useful tool in obtaining good quantitative estimates for some phase boundaries as compared to the usual mean-field theories. In addition, it allows one to estimate critical exponents for the two-dimensional model by means of a standard procedure. The present approach can also be easily extended to treat the more general three-dimensional ANNNI model in which one has a different exchange coupling J_0 in planes perpendicular to the axial direction. In this case, differing from the usual mean-field theories, the location of the Lifshitz point depends on the ratio J_0/J_1.

It should be mentioned that wider clusters could also be considered. In comparison to other methods, in which only the largest and second largest eigenvalues are required (Beale *et al* 1985), in the present approach it is necessary to evaluate both all eigenvalues and all eigenvectors of the related transfer matrix. Most importantly, the magnetisation per spin for clusters wider than the double chain is no longer connected to the usual susceptibilities, thus not enabling us to use the procedure recently proposed by Pesh and Kroemer (1985) for calculating $\chi_N(q)$ for $N \geq 3$. Moreover, a very slow convergence to the exact results should be expected as the width of the infinite strips is made larger, as recently verified for the triple chain in the Ising limit (Plascak and Silva 1986). We therefore conclude that the present choice of clusters represents the most feasible one within a MFRG calculation on the ANNNI model.

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