Ising model with third-neighbour interactions on the Cayley tree

1987 J. Phys. A: Math. Gen. 20 1621

(http://iopscience.iop.org/0305-4470/20/6/043)

J. Phys. A: Math. Gen. 20 (1987) 1621-1625. Printed in the UK

COMMENT

Ising model with third-neighbour interactions on the Cayley tree

J G Moreira† and S R Salinas‡

† Departamento de Física, Universidade Federal de Minas Gerais, CP 702, 30000, Belo Horizonte, MG, Brazil
‡ Instituto de Física, Universidade de São Paulo, CP 20516, 01498, São Paulo, Brazil

Received 23 June 1986

Abstract. We formulate the Ising model with competing first-, second- and third-neighbour interactions along the branches of a Cayley tree, in the infinite coordination limit, as a three-dimensional non-linear mapping problem. The phase diagrams display a Lifshitz point and many modulated phases. The introduction of third-neighbour interactions affects mainly the low-temperature region of the phase diagrams.

The axial next-nearest-neighbour Ising (ANNNI) model, which consists of an Ising model with competing interactions between first and second neighbours along an axial direction, has been introduced to account for the existence of modulated structures in several physical systems. For instance, it has been used to study magnetic compounds such as CeSb (Rossat-Mignod *et al* 1980), ferroelectrics such as $NaNO_2$ (Yamada *et al* 1963, Selke and Duxbury 1984) and polytypes (Price and Yeomans 1984).

The layer-by-layer mean-field solutions of the ANNNI model (Bak and van Boehm 1980, Yokoi *et al* 1981) are particularly hard to analyse in the modulated region of the phase diagram. However, if we consider an analogue of this model, with competing interactions between first and second neighbours along the branches of a Cayley tree (Vannimenus 1981), it is possible to write the solution of the statistical problem in terms of a set of three first-order recursion relations. Yokoi *et al* (1985) realised that these recursion relations are considerably simplified in the infinite coordination limit (that is, for J_1, $J_2 \to 0$ and $z \to \infty$, with zJ_1 and z^2J_2 fixed, where J_1 and J_2 are the exchange interactions between first and second neighbours, respectively, and z is the coordination of the tree). It should be mentioned that the infinite coordination limit of the Cayley tree reproduces the mean-field results for the nearest-neighbour Ising model on a Bravais lattice of the same coordination (Thompson 1982). The simple second-order recursion relations of Yokoi *et al* (1985), which can be analysed in great detail, give rise to the main quantitative features of the phase diagram corresponding to the ANNNI model.

In a recent paper, Yamada and Hamaya (1983) proposed an Ising model with axial interactions between first, second and third neighbours to study the commensurate and incommensurate structures in ferroelectric systems of the type A_2XB_4. Mean-field and low-temperature series analyses of this model have been carried out by Selke *et al* (1985) and Barreto and Yeomans (1985). In the present paper, we consider an Ising model on a Cayley tree of coordination z, with exchange interactions between first (J_1), second (J_2) and third (J_3) neighbours along the branches of the tree. Although not entirely similar, this is certainly the counterpart on a tree of the Ising model considered by Yamada and Hamaya. As in the case of the ANNNI model, we take full advantage of the infinite coordination limit (J_1, J_2, $J_3 \to 0$, $z \to \infty$, with zJ_1, z^2J_2 and z^3J_3 fixed) to obtain a simple third-order recursion relation for the effective layer magnetisation per spin. A similar model, with finite z, which leads to a higher-order system of equations, had been previously studied by Silva and Coutinho (1985).

Using a decimation procedure to eliminate the spins on the outer shells of the Cayley tree (Inawashiro *et al* 1983) we obtain a system of recursion relations. In the infinite coordination limit, this system is reduced to the set of third-order relations

$$X_n = \frac{H}{k_B T} + \frac{zJ_1}{k_B T} \tanh X_{n-1} + \frac{z^2 J_2}{k_B T} \tanh X_{n-2} + \frac{z^3 J_3}{k_B T} \tanh X_{n-3} \tag{1}$$

where H is the external field, T the absolute temperature, k_B Boltzmann's constant and X_n is an effective field induced in the nth shell of the tree. If we define the effective magnetisation per spin in the nth shell, $m_n = \tanh X_n$, it is possible to rewrite (1) in the more convenient form

$$m_n = \tanh[t^{-1}(m_{n-1} - pm_{n-2} - rm_{n-3}) + h] \tag{2}$$

where $t = k_B T/zJ_1$, $p = -z^2J_2/zJ_1$, $r = -z^3J_3/zJ_1$ and $h = H/k_BT$. Equation (2) is similar to the mean-field equation of state for the ANNNI model (see, for example, Jensen and Bak 1983). In the present case, however, there are no interactions between spins on the same shell. Also, the hierarchical character of the Cayley tree breaks the translational invariance of the model. It should be remarked that it is straightforward to write a generalisation of (2) to account for the inclusion of fourth-, fifth-, etc, neighbour interactions along the branches of the tree.

The paramagnetic lines of the phase diagram are obtained from the analysis of the stability of the paramagnetic fixed point of (2) ($m_n^* = 0$, for all n, with $H = 0$). For $r > -\frac{1}{3}$, we obtain a number of analytical results. In the t-p space, there is a second-order paramagnetic-ferromagnetic transition for $t + p + r = 1$, with $p < (1-3r)/2$, and a paramagnetic-modulated transition for $p = t - r(1+r)/t$, with $p > (1-3r)/2$. Thus, for $r > -\frac{1}{3}$, the Lifshitz point is located at $p = (1-3r)/2$ and $t = (1+r)/2$. Along the paramagnetic-modulated second-order transition line, the critical wavevector is given by $\cos q_c = (1+r)/2t$. For $r < -\frac{1}{3}$, on the other hand, we have to resort to a numerical analysis in order to study the stability conditions.

The boundaries between the modulated phases shown in figure 1, for $r > 0$, and in figure 2, for $-\frac{1}{3} < r < 0$, have been obtained from a numerical analysis of (2) in zero field. For given values of t, p and r, the equilibrium configuration is found by repeated iterations of the recursion relation, with given initial values for m_0, m_1 and m_2. Besides the trivial paramagnetic ($m^* = 0$) and ferromagnetic ($m^* \neq 0$) fixed points, the effective magnetisation may flow to (i) a well defined periodic cycle ($m_{n+L}^* = m_n^*$), which corresponds to a commensurate modulated phase with period L; (ii) a one-dimensional orbit, which is associated with an incommensurate phase (or, within the precision of the numerical calculation, with a commensurate phase of a very large period) and (iii) a strange attractor with a fractal character, which is associated with a possible chaotic phase. In figures 1 and 2 we show the main commensurate phases only. The principal wavevector of a commensurate phase of period L, in units of 2π, is given by $q = (l+1)/2L$, where l indicates the number of changes of sign of the effective magnetisation in the period L. In the hatched regions of figures 1 and 2, the magnetisation can flow either to a ferromagnetic or to a modulated fixed point, depending on the initial

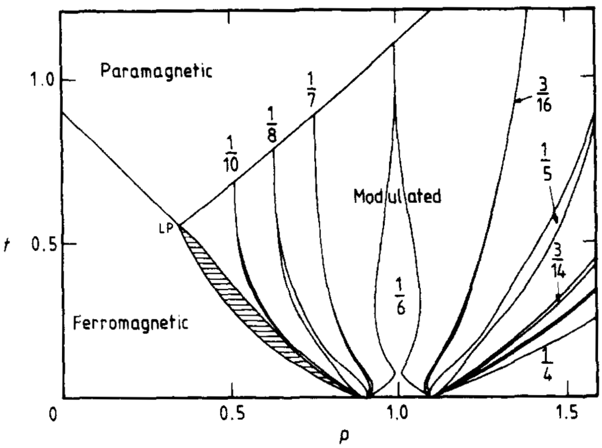

Figure 1. Global t-p phase diagram ($t = k_B T/zJ_1$, $p = -z^2J_2/zJ_1$) of the Ising model on the Cayley tree, in the infinite coordination limit, with $r = 0.1$ ($r = -z^3J_3/zJ_1$). We show the paramagnetic, ferromagnetic and modulated regions and the Lifshitz point (LP). The main commensurate phases are indicated by their corresponding principal wavenumbers. In the hatched region there is the possibility of the coexistence between ferromagnetic and modulated phases.

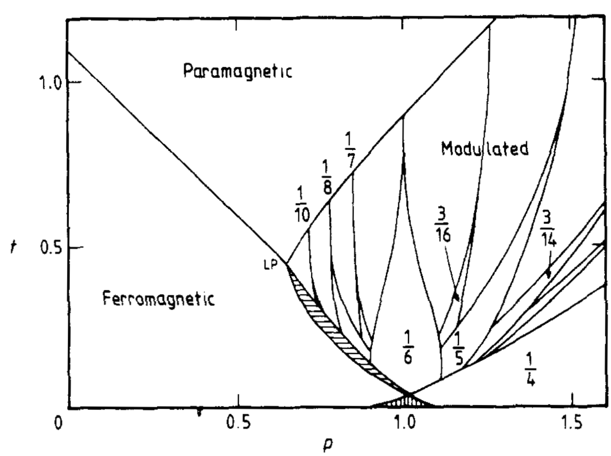

Figure 2. Global t-p phase diagram with $r = -0.1$. At low temperatures, near $p = 1$, the hatched region corresponds to the occurrence of either ferromagnetic or $\frac{1}{4}$ phases, depending on the initial conditions of the mapping.

conditions. These results are then interpreted as the indication of the occurrence of a first-order boundary between the ferromagnetic and the modulated regions (see, for example, de Oliveira and Salinas 1985).

It is interesting to compare figures 1 and 2 with the phase diagram for the case $r = 0$ (see figure 1 in Yokoi *et al* (1985)). For high temperatures, these phase diagrams are all similar. For low temperatures, however, there are sensible differences, which are related to the new ground state defined by the presence of the third-neighbour interactions. The ground state of the cubic lattice, shown in figure 1 of Selke *et al* (1985), exhibits, for $r > 0$, two multiphase points, corresponding to the ferromagnetic-$\frac{1}{16}$ and the $\frac{1}{6}$-$\frac{1}{4}$ phase transitions. For sufficiently small $r < 0$, at low temperatures, the ferromagnetic-$\frac{1}{4}$ transition is first order and there is no multiphase point in the ground state of the cubic lattice. Similar features are present in the models defined on the Cayley tree. At low temperatures, for $r<0$, the phase diagram of figure 2 shows a hatched region, which corresponds to either a ferromagnetic or a $\frac{1}{4}$ phase, depending on the initial conditions. For $m_0 = m_1 = m_2 = 1$, the mapping flows to a ferromagnetic fixed point. However, if the sign of any initial effective spin magnetisation is changed, there is a flow to a $\frac{1}{4}$ phase. This is a clear indication of the occurrence of a first-order phase transition.

For $r>0$, with fixed t, the wavevector q increases with p and gives rise to a standard devil's staircase, as in the $r=0$ case. With increasing temperature, the width of the main commensurate phases begins to decrease, then increases again, and then decreases as in the $r=0$ case. For $r<0$, the behaviour of the wavevector q is quite unusual at low temperatures. The convergence of the iterative process is slow and, for fixed t, q does not increase with p in a regular fashion. The influence of the initial conditions is overwhelming and we do have first-order transitions between the main commensurate phases. At higher temperatures, the phase diagram again exhibits its usual properties.

The qualitative differences between our calculations on the Cayley tree and the mean-field results of Selke *et al* (1985) are analogous to the differences between the phase diagrams of the Vannimenus model in the infinite coordination limit (Yokoi *et al* 1985) and the usual mean-field ANNNI model on a cubic lattice. On the Cayley tree, the Lifshitz point corresponds to an angular junction of the second-order para-ferromagnetic and paramagnetic-modulated, and the first-order ferromagnetic-modulated, transition lines. At low temperatures, on the Cayley tree, the lines which spring from the multiphase point do not show the characteristic infinite tangent as in the ANNNI model. Also, the sequence of commensurate phases at low temperatures turns out to be different. However, preliminary calculations for a Cayley tree with the inclusion of some first-neighbour ferromagnetic interactions between spins belonging to the same shells indicate that the infinite tangent, as well as the sequence of commensurate phases, may change towards the characteristic features of the ANNNI model.

In conclusion, the addition of third-neighbour interactions has not changed the main features of the phase diagram of the Vannimenus model in the infinite coordination limit. The modifications at low temperatures may be relevant to signal the extra care which has to be taken in the interpretation of experimentally interesting systems.

We acknowledge helpful conversations with Sergio G Coutinho.

References

Bak P and von Boehm J 1980 *Phys. Rev.* B **21** 5297
Barreto M and Yeomans J 1985 *Physica* **134A** 84
de Oliveira M J and Salinas S R 1985 *Rev. Bras. Fis.* **15** 189
Inawashiro S, Thompson C J and Honda G 1983 *J. Stat. Phys.* **33** 419
Jensen M and Bak P 1983 *Phys. Rev.* B **27** 6853
Price G D and Yeomans J M 1984 *Acta Crystallogr.* B **40** 448
Rossat-Mignod J, Burlet P, Bartholin H, Vogt O and Lagnier R 1980 *J. Phys. C: Solid State Phys.* **13** 6381
Selke W, Barreto M and Yeomans J 1985 *J. Phys. C: Solid State Phys.* **18** L393
Selke W and Duxbury P M 1984 *Z. Phys.* B **57** 49
Silva C R and Coutinho S 1985 unpublished

Thompson C J 1982 *J. Stat. Phys.* **27** 441
Vannimenus J 1981 *Z. Phys.* B **43** 141
Yamada Y and Hamaya N 1983 *J. Phys. Soc. Japan* **52** 3466
Yamada Y, Shibuya I and Hoshino S 1963 *J. Phys. Soc. Japan* **18** 1594
Yokoi C S O, Coutinho-Filho M D and Salinas S R 1981 *Phys. Rev.* B **24** 4047
Yokoi C S O, de Oliveira M J and Salinas S R 1985 *Phys. Rev. Lett.* **54** 163