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1989 J. Phys.: Condens. Matter 1 1849

(http://iopscience.iop.org/0953-8984/1/10/006)

J. Phys.: Condens. Matter 1 (1989) 1849–1854. Printed in the UK

Mean-field theory evidence for a Devil's staircase in the three-state chiral Potts model

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Received 12 May 1988, in final form 22 August 1988

Abstract. We study the mean-field theory of the three-state chiral Potts model with isotropic next-nearest-neighbour interactions. Numerical analysis of the mean-field equations shows evidence for an infinite cascade of phases arranged in a Devil's staircase. This result agrees with earlier predictions of the low-temperature expansion technique.

One problem in the statistical physics of spin–lattice systems is the form of low-temperature phase diagrams for layered systems. Best known examples are the ANNNI model and the three-state chiral Potts model. Their phase diagrams have been studied by several workers (cf [1–5] for the ANNNI and [4, 6–12] for the three-state chiral Potts model) and exhibit an infinite number of modulated phases arranged essentially in a stepwise structure. Recently a new version of the three-state chiral Potts model with isotropic NNN interaction has been proposed [13] which has a different phase diagram. The low-temperature expansion (LTE) analysis of this model shows that modulated phases are arranged in an infinite cascade resembling a Devil's staircase. A similar feature has been found in [5] for the ANNNI model in a non-zero magnetic field.

In this paper the mean-field (MF) theory of the three-state chiral Potts model with NNN interactions is reported. We restrict attention to the region where the LTE analysis showed the existence of an infinite cascade of phases. First, we define the model. Then we discuss the numerical analysis of the modulated phases. To conclude, the results are compared with predictions of the LTE technique.

Let us consider a simple cubic lattice with base vectors $\{e_1, e_2, e_3\}$. The spin at each lattice point can assume the values 0, 1, 2 (with addition modulo 3). The three-state Potts model with NNN interaction, first introduced in [13], is described by the Hamiltonian

$$\mathscr{H} = -(1+x)\sum_{a}\sum_{i=0}^{2}\sum_{k=1}^{3} P_a^i P_{a+ek}^{i+1} - \sum_{NNN}\sum_{i=0}^{2} P_a^i P_b^i. \tag{1}$$

Here P_a^i is the projection on value i at the point $\boldsymbol{a}$; if S is a spin configuration, then $P_a^i(S) = 1$ is $S_a = i$, and $P_a^i = 0$ otherwise. The second term represents the NNN ferromagnetic interaction, while the first term describes the 'chiral' coupling favouring configurations with $S_{a+e_k} = S_a + 1 \pmod 3$. A similar model but with chiral coupling only has been studied in [7]. The Hamiltonian $\mathscr{H}$ is invariant with respect to uniform transformations of spins, $S \to S + k \pmod 3$, and also with respect to rotations of the lattice about the axis (1, 1, 1). It is not invariant with respect to reflections in planes perpendicular to (1, 1, 1). Such planes will be called layers. Layers will be numbered in the

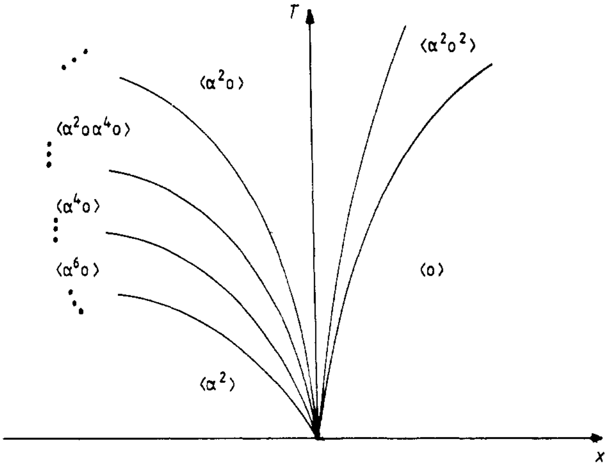

Figure 1. The general form of the phase diagram found by the LTE technique. Ellipses (. . .) between phases denote an infinite number of intermediate phases.

order of their appearance counting from the origin.

A spin S_a in the layer L_n is coupled ferromagnetically with its six NNN spins lying in L_n. Thus each ground state G is constant in any layer and can be described by a sequence of spin values $\{G_n\}$, with G_n being the value of G in the nth layer. Furthermore, S_a is coupled ferromagnetically with its three NNN spins in layers L_{n-2} and L_{n+2}, and it interacts 'chirally' with three NN spins in layers L_{n-1} and L_{n+1}. The competition between these two inter-layer interactions leads to the following restrictions on the sequence $\{G_n\}$.

(i) If $x < 0$ then, for any n, $G_{n-1} = G_{n+1} \neq G_n$. The configuration on the layer L_n (and the layer L_n) is called α.

(ii) If $x > 0$ then, for any n, $G_{n+1} = G_n + 1 = G_{n-1} + 2 \pmod 3$ (the chiral ordering). L_n is called an o layer.

(iii) If $x = 0$, then G can contain both α and o layers, with the restriction that any two o layers are separated by an even number (including zero) of α layers.

Thus any ground state G can be described symbolically by a sequence of o and $\alpha\alpha \equiv \alpha^2$. A periodic ground state G corresponds to a periodic sequence A, and

$$(\text{period of } G) = n(A) \times (\text{length of } A). \tag{2}$$

Here $n(A) = 1$ if the number of o symbols in A equals zero modulo 3, and $n(A) = 3$ otherwise.

For the model (1) described above, the LTE technique predicts the phase diagram in figure 1. For $x > 0$, there are three phases: $\langle \mathrm{o} \rangle$ (right chiral), $\langle \alpha^2\mathrm{o} \rangle$ (corresponding to the periodic repetition of the spin sequence 010121202) and $\langle \alpha^2\mathrm{o}\alpha^2\mathrm{o}^2 \rangle$. For x negative, low temperatures are occupied by $\langle \alpha^2 \rangle$ and high temperatures by $\langle \alpha^2\mathrm{o} \rangle$. The intermediate-temperature region is filled up by an infinite collection of phases forming the structure resembling the Devil's staircase (figure 2).

In the MF approximation, we assume that the thermal average of the projection P_a^i is constant through any layer L_n, i.e. $\langle P_a^i \rangle \coloneqq \pi_n^i$ if a lies in L_n. The MF theory of the model (1) is described by the Hamiltonian

$$\mathcal{H}_{\mathrm{MF}} = -\sum_{n=-\infty}^{\infty} \sum_{a \in L_n} \sum_{i=1}^{2} (P_a^i - \pi_n^i) H_n^i \tag{3}$$

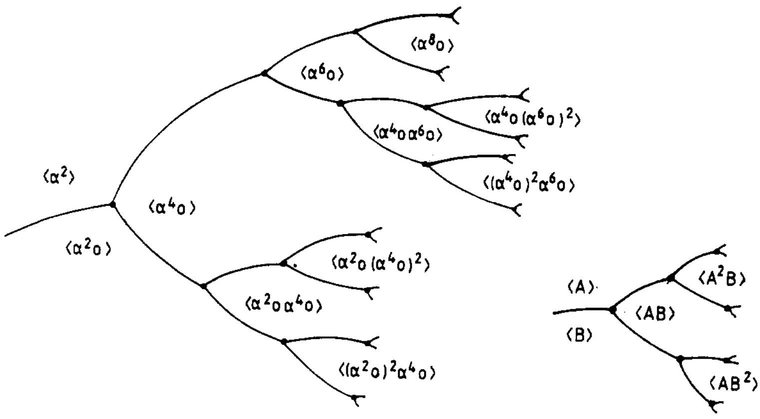

Figure 2. Schematic representation of intermediate phases in figure 1 for x negative. Every boundary bifurcates in some order into two boundaries and a new phase appears at its locus. The scheme is continued in the way shown on the right-hand side of the diagram.

$$H_n^i = 3(1+x)(\pi_{n+1}^{i+1} + \pi_{n-1}^{i-1}) + 3\pi_n^i + 3(\pi_{n+2}^i + \pi_{n-2}^i). \tag{4}$$

Thermal averages have to satisfy the self-consistency equation

$$\pi_n^i = \exp(H_n^i/T)/[\exp(H_n^0/T) + \exp(H_n^1/T) + \exp(H_n^2/T)]. \tag{5}$$

The system of equations (4) and (5) has a solution $\pi_n^i = \frac{1}{3}$, which corresponds to the paramagnetic phase. To find other phases, we used a numerical procedure first introduced in [3] for the ANNNI model and then utilised in [6] to study the three-state chiral Potts model. First, we assume that the system consists of N layers with periodic boundary conditions. Our calculations were done for $N \leqslant 27$. Starting for fixed N from some initial conditions (see below) which enter into (4), one finds new spin configurations from (5). Then the procedure is repeated until the spin configurations obtained in two consecutive steps coincide to within some fixed accuracy. The average free energy per spin is calculated for every solution from

$$F = \frac{1}{N} \sum_{n=1}^{N} \left[\frac{1}{2} \sum_{i=0}^{2} \pi_n^i H_n^i - T \ln \left(\sum_{i=0}^{2} \exp(H_n^i/T) \right) \right]. \tag{6}$$

The solution with the least free energy determines the phase of the system for given temperature T and perturbation parameter x. Phases were identified in the following way. For each solution of (4) and (5), we define the sequence of spin values

$$S_n = \pi_n^1 + 2\pi_n^2 \qquad n = 1, \ldots, N.$$

We say that the system is in the phase G which is a small variation of the ground state G if

$$|S_n - G_n| \leqslant 0.25 \qquad \left(\frac{1}{N} \sum_{i=1}^{N} (S_n - G_n)^2 \right)^{1/2} < 0.1. \tag{7}$$

Away from the transition to the paramagnetic phase, all minimal free-energy solutions could be associated with some ground state.

For fixed N, the initial conditions were taken to be

$$S_n = [3qn/N] (\mathrm{mod}\ 3) \qquad \pi_n^i = \begin{cases} 1 & \text{if } S_n = i \\ 0 & \text{otherwise} \end{cases} \tag{8}$$

for all $q = 1, \ldots, N$. Here $[a]$ is the integer part of a. We were motivated in this choice by previous work [3, 6]. Since ground states of (1) are highly irregular compared with the ground states of the ANNNI or the three-state chiral Potts model, we do not expect that phases can be simply related to some mean wavevector q/N. However, it turned out that for most N the set of initial conditions (8) is complete in the following sense. If there exists a ground state G with period N and such that $n(A) = 1$ in (2), then the solution with minimal free energy is close to G in the sense of definition (7). If $n(A) = 3$, then the structure of the corresponding ground state is too complicated and the set of initial conditions (8) does not produce an appropriate solution. For these values of N, we added new initial conditions described by respective ground states:

$$S_n = G_n \qquad n = 1, \ldots N \qquad \pi_n^i = \begin{cases} 1 & \text{if } S_n = i \\ 0 & \text{otherwise} \end{cases} \tag{9}$$

Solutions obtained from (9) had free energy smaller than those from (8), which justifies our procedure.

Calculations were performed in three main steps. First, the temperature range was scanned at large intervals ($\Delta T = 0.1$). The upper temperature bound was determined from the condition (7). Above this, the convergence of our procedure was very poor and we did not investigate this region. In all cases, $\langle \alpha^2 \rangle$ was found to be the low-temperature phase. For $x > -0.08$, the high-temperature phase was $\langle \alpha^2 \mathrm{o} \rangle$, which was for $x \leqslant -0.08$ replaced by $\langle (\alpha^2 \mathrm{o})^2 \alpha^4 \mathrm{o} \rangle$ and for $x \leqslant -0.09$ by $\langle \alpha^2 \mathrm{o} \alpha^4 \mathrm{o} \rangle$. In the second step, the region between $\langle \alpha^2 \mathrm{o} \rangle$ and a high-temperature modulated phase was studied more closely with temperature steps $\Delta T = 0.01$, and with an accuracy for projection averages of 10^{-5}. The following intermediate phases appeared: $\langle \alpha^6 \mathrm{o} \rangle$, $\langle \alpha^4 \mathrm{o} \rangle$, $\langle \alpha^4 \mathrm{o} \alpha^2 \mathrm{o} \rangle$ and $\langle (\alpha^2 \mathrm{o}^2 \alpha^4 \mathrm{o} \rangle$. Finally, the boundaries between these phases were investigated with temperature steps ΔT of 10^{-5}–10^{-6} and an accuracy of 10^{-9}.

The phase diagram obtained in the second step is shown in figure 3. In the third step, additional phases were found (figure 4). They occupy regions of widths much smaller than do the dominating phases of the second step. The phase diagram has all the qualitative features predicted by the LTE technique. The only phases with period less than 27 which are missing are $\langle \alpha^8 \mathrm{o} (\alpha^6 \mathrm{o})^2 \rangle$ (period 23) and $\langle (\alpha^8 \mathrm{o})^2 \alpha^6 \mathrm{o} \rangle$ (period 25). The LTE technique predicts here that regions occupied by these phases are of the order of 10^{-28} compared with the neighbouring phases (cf. [13]). Although one cannot expect the LTE technique to give correct values at intermediate temperatures, the discussed regions are probably extremely narrow and will not show up with the assumed width of temperature steps of 10^{-6}. In one case ($x = -0.08$), we carried out the more refined analysis of the boundary between $\langle \alpha^8 \mathrm{o} \rangle$ and $\langle \alpha^6 \mathrm{o} \rangle$ with temperature steps of 10^{-8}. By linear interpolation of free energies (6) we found the phase $\langle (\alpha^6 \mathrm{o})^2 \alpha^8 \mathrm{o} \rangle$ in the region of width 10^{-9}. We did not go so far with the analysis in other cases.

Obviously the MF theory of the model (1) is complete only if one considers all values of N up to infinity. However, we believe that figures 3 and 4 show the beginning of the infinite cascade in figure 2. Further evidence could be obtained if one extends the calculations to structures with larger periods, but probably numerical analysis would quite soon become ineffective because of the very small variations in the quantities involved (e.g. free energy (6)).

In this paper, we have presented the MF theory of the three-state Potts model with NNN interactions. The numerical solution of the MF equations shows a collection of phases which are arranged in a cascade resembling a Devil's staircase. This confirms results of the LTE treatment of the model.

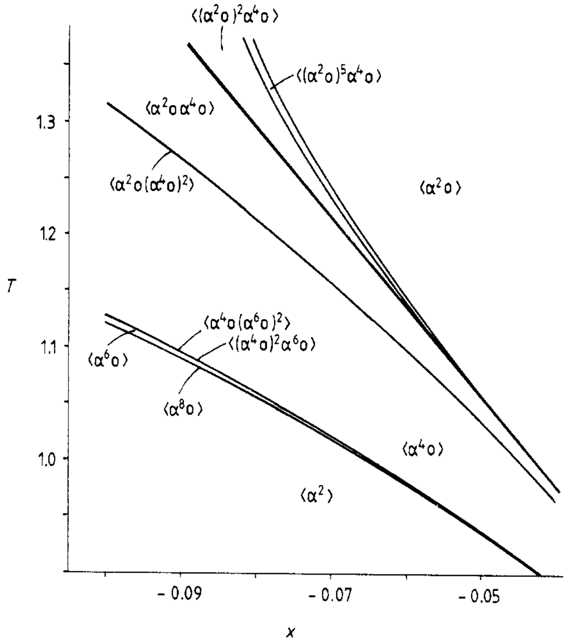

Figure 3. The phase diagram in the MF approximation for x negative. Narrow regions in the vicinity of the boundaries are occupied by additional intermediate phases (cf figure 4).

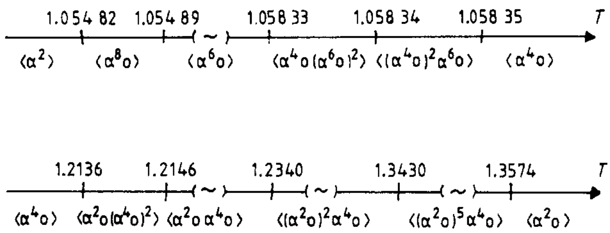

Figure 4. Intermediate phases between (top) $\langle\alpha^2\rangle$ and $\langle\alpha^4\mathrm{o}\rangle$, (bottom) $\langle\alpha^4\mathrm{o}\rangle$ and $\langle\alpha^2\mathrm{o}\rangle$ for $x = -0.08$.

Acknowledgments

This work has been supported by the Institute of Low Temperature and Structural Research of The Polish Academy of Sciences from the resources of the Central Programme for Fundamental Research: Structure, Phase Transitions and Properties of Molecular Systems and Condensed Matter. Numerical calculations were performed on an IBM PC/AT.

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