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1990 J. Phys.: Condens. Matter 2 8599

(http://iopscience.iop.org/0953-8984/2/43/006)

J. Phys.: Condens. Matter **2** (1990) 8599–8613. Printed in the UK

The low-temperature phase diagram for the q-state Potts model with next-nearest-neighbour interaction

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Received 2 November 1989, in final form 17 April 1990

Abstract. The phase diagram for the q-state Potts model is constructed by means of the low-temperature expansion technique. An infinite set of phases appears, with the bifurcating structure resembling the complete Devil's staircase.

1. Introduction

Classical spin systems with a layered structure of the ground state have received considerable attention for some time. The best known example is the ANNNI model [1], which has been studied by a variety of methods (cf the review by Selke [2]). Another representative is the q-state chiral clock (CC) model [3, 4]. Phase diagrams for these two systems exhibit infinite sequences of phases springing from a zero-temperature multiphase critical point. The form of such a phase diagram can be described as an incomplete Devil's staircase: the transition between high-temperature and low-temperature bulk phases occurs through a sequence of periodic structures with increasing periods. In the more complicated form, the complete Devil's staircase, any two phases are separated by an infinite collection of structures with higher periodicity. The phase diagram of this type has been found in the ANNNI model with a magnetic field [5].

In this report we present results of the low-temperature expansion (LTE) analysis of a modified version of the q-state CC model. In the formulation of the three-state CC model by Huse [3], the Hamiltonian is defined on the oriented simple cubic lattice by competing nearest-neighbour (NN) interactions: ferromagnetic and 'chiral'. The latter forces spins along any (oriented) axis to have values $0, 1, 2, \ldots$ (modulo 3). In this form the model cannot be analysed by the LTE technique and hence it was modified [6]: competing ferromagnetic and chiral interactions were preserved along some chosen axis while in the remaining directions, ferromagnetic bonds were imposed. The phase diagram for this model was studied by Yeomans and Fisher [6] (three-state CC) and by Yeomans [7] (q-state CC). In both cases the incomplete Devil's staircase was found.

In our version we keep the NN chiral bonds, but replace the NN ferromagnetic interaction by the next-nearest-neighbour (NNN) one. The original symmetry of the system is thus preserved. The Hamiltonian has an infinite number of ground states and yet the LTE technique can be applied. Spin is allowed to assume values $0, 1, \ldots, (q-1)$. This model (for $q = 3$) was first introduced in [8], where it served as an example for the LTE application to layered systems. Here we present a full account of the LTE calculations

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for general q. The resulting phase diagram has the form of a complete Devil's staircase. This has been confirmed to some extent by the numerical analysis of the mean-field theory for the model [9]. It is worth noting that the renormalisation group treatment of the original model [3] produced the phase diagram with some features of the complete Devil's staircase.

Since the Hamiltonian of the system has an infinite number of ground states, some inductive argument has to be used. We apply the method described in [8]. The paper is divided into two main parts: in section 2 steps of the inductive pattern are outlined and results are presented while the derivations of the expansion coefficients are deferred to section 3. The phase diagram is shown in figures 1 and 2 and is identical to the phase diagram for $q = 3$ (cf [8]). A brief discussion of results (section 4) concludes the report.

2. The phase diagram construction

2.1. The model

Let us consider the simple cubic lattice $\mathbb{Z}^3$ with base vectors e_1, e_2, e_3 being the edges of a cube. In every lattice point, spin can assume values $0, 1, 2, \ldots, q-1$. The Hamiltonian is

$$H = -J_1 \sum_{a\in\mathbb{Z}^3} \sum_{i=0}^{q-1} \sum_{k=1}^{3} P_a^i P_{a+e_k}^{i+1} - \tfrac{1}{2}J_2 \sum_{(a,b)} \sum_{i=1}^{q-1} P_a^i P_b^i \tag{2.1}$$

with the second summation over next nearest neighbours (NNN). Here P_a^i is the projection on the spin value i at the lattice point a: $P_a^i(X) = 1$ if $X_a = i$, zero otherwise. Both J_1 and J_2 are positive. The first term in (2.1) is the chiral interaction (cf [3]), while the second one is the ferromagnetic coupling. The Hamiltonian (2.1) is invariant with respect to rotations about the (1, 1, 1) axis and to uniform spin rotations: $X_a \to X_a + m \pmod q$. It is not invariant with respect to reflections in any lattice plane perpendicular to (1, 1, 1). Any such plane will be called a layer. Layers will be numbered in the order of their appearance, starting from the origin.

2.2. Ground states

Ground states of the model can be easily found if one defines new interactions Φ_Δ, $\Phi_\perp$:

$$\Phi_{\Delta,J_1,J_2} = \sum_{i=1}^{q-1} [-\tfrac{1}{4}J_1(P_a^i P_{a+e_k}^{i+1} + P_{a+e_k}^i P_{a+e_k+e_j}^{i+1}) - \tfrac{1}{2}J_2 P_a^i P_{a+e_k+e_j}^i] \tag{2.2a}$$

where $k \neq j$; $k, j = 1, 2, 3$, and

$$\Phi_{\perp,J_2} = -\tfrac{1}{2}J_2 \sum_{i=1}^{q-1} P_{a+e_k}^i P_{a+e_j}^i. \tag{2.2b}$$

Then

$$H = \sum_\Delta \Phi_\Delta + \sum \Phi_\perp \tag{2.3}$$

with the second summation over all NNN pairs lying in the same layer. Values of Φ_Δ for various configurations on a triangle $\{a, a + e_k, a + e_k + e_j, j \neq k\}$ are the following (we

fix $X_a = 0$, $X_{a+e_k} = m$, $X_{a+e_k+e_j} = k$):

$$k = 0, m = 1, q-1: -(J_1 + J_2)/4 \qquad k = 2, \quad m \neq 1: \qquad 0$$

$$k = 0, m \neq 1, q-1: -J_1/4 \qquad k \neq 0, 2, m = 1, k-1: -J_1/4$$

$$k = 2, m = 1: \qquad -J_1/4 \qquad k \neq 0, 2, m \neq 1, k-1: 0.$$

For configurations with $X_a \neq 0$ use the spin rotation. Obviously (2.2) is equivalent to the original interaction, so it has the same ground states. They are the following:

(i) Throughout any fixed layer, values of spins are the same.

(ii) If $J_1 > J_2$, then in any three consecutive layers L_{n-1}, L_n, L_{n+1} spin values are $m-1, m, m+1 \pmod q$. We say in short that L_n is the o layer.

(iii) If $J_1 < J_2$, then spin values in L_{n-1}, L_n, L_{n+1} are $m, m+1, m \pmod q$ (the α layer) or $m, m-1, m \pmod q$ (the β layer).

(iv) If $J_1 = J_2$, then any of the above configurations on triples of layers is allowed, with obvious restrictions that the α layer has to be followed by the β layer while o and β layers cannot be followed by the β layer.

The most interesting situation occurs close to the multiphase point $J_1 = J_2$. To study this region we split the Hamiltonian (2.1) into $H_0 = H(J_1 = J_2)$ and the perturbation L:

$$L = -\delta \sum_a \sum_{k=1}^{3} \sum_{i=0}^{q-1} P_a^i P_{a+e_k}^{i+1} \qquad \delta = J_1 - J_2. \tag{2.4}$$

Each ground state of H_0 (which from now on will be referred to as the ground state) can be uniquely described by its value in the zeroth layer (L_0) and by a sequence of symbols α, β or o defining types of consecutive layers. Ground states that differ only by the spin value at the origin are related by a symmetry of the Hamiltonian (a spin rotation) and can be identified. In the low-temperature expansion (LTE) technique we consider periodic ground states only which correspond to periodic sequences of symbols. The periodic repetition of the sequence A will be denoted by $\langle A \rangle$.

Example. The periodic repetition $\langle \alpha\beta o \rangle$ of the sequence $\alpha\beta 0$ defines q ground states. One of them is the periodic repetition of $01012123234 \ldots (q-2)(q-1)0(q-1)$.

2.3. Structural variables

Let G be a ground state and A any finite sequence of symbols α, β or 0. In N consecutive layers A appears $N_A(G) = Nl_A(G)$ times (modulo boundary terms) as a sub-sequence of G. In the limit of infinite N, $l_A(G)$ is the density of A in G. Following [10], it will be called a *structural variable*. Since G is periodic, $l_A(G)$ is well defined.

Example. $l_{\alpha\beta o}(\langle \alpha\beta o \rangle) = 1/3$, $l_{\alpha\beta o}(\langle \alpha\beta\alpha\beta o\alpha\beta o \rangle) = 1/4$.

Structural variables satisfy structural relations:

$$l_A(G) = \sum_{|B|=b} l_{AB}(G) = \sum_{|B|=b} l_{BA}(G) \tag{2.5}$$

where $|B|$ is the length of B, and AB denotes A followed by B. In particular,

$$l_\varnothing(G) = 1 = l_\alpha(G) + l_\beta(G) + l_o(G). \tag{2.6}$$

Structural variables allow one to parametrise with G various quantities appearing in

the LTE technique. For example, let us consider the average energy per lattice site in the ground state G:

$$e_G = -3J_2 - \tfrac{3}{2}(J_1 + J_2)[l_\alpha(G) + l_\beta(G)] - 3J_1 l_0(G).$$

Using structural relations (2.6) one can rewrite the above in the form:

$$e_G(\delta) = e_G(0) - \tfrac{3}{2}\delta l_0(G) = \text{const} - \tfrac{3}{2}\delta l_0(G). \tag{2.7}$$

2.4. The low-temperature expansion of the pressure

Let G be a ground state. A spin configuration X is called an *excitation* of G if X differs from G in a finite number of lattice points, and

$$E(X) \equiv \sum_{\Delta} [\Phi_{\Delta, J_1 = J_2}(X) - \Phi_{\Delta, J_1 = J_2}(G)] + \sum [\Phi_\perp(X) - \Phi_\perp(G)] \geqslant 0. \tag{2.8}$$

Since both Φ_Δ and $\Phi_\perp$ attain their minima at G, the inequality is in fact strict.

The main object in the LTE technique is the expansion of the pressure in boundary conditions given by a ground state G:

$$p^G(\beta, \delta) = -e_G(\delta) + (1/\beta) \sum_{i=1}^{\infty} n_i^G(\beta\delta)\, e^{-\beta E_i} \tag{2.9}$$

where $1/\beta = kT$, e_G is given by (2.7) and E_i is the sum of excitation energies (2.8). The construction of expansion coefficients n_i^G has been thoroughly described elsewhere [11] and it will be briefly reviewed in section 3.1. For further discussion it is important that each n_i^G can be written as a linear combination of structural variables [8, 10]:

$$n_i^G(\beta\delta) = \sum_{|A| \leqslant r} a_{i,A}(\beta\delta) l_A(G) \tag{2.10}$$

where $a_{i,A}$ is independent of G. The restriction on the length of sequences entering into (2.10) comes from the finiteness of the interaction range and from proposition 2 of section 3.1.

Except for very specific cases [12], nothing is known about the convergence of the series (2.9). The standard procedure is to cut it at some term N and use truncated pressures p_N^G to construct the phase diagram in order N. The truncated pressure p_N^G corresponds to the phase G in which typical spin configurations are very close to the ground state G. The line of coexistence (in order N) of phases G_1 and G_2 is the curve $\delta(\beta)$ for which

$$p_N^{G_1}(\beta, \delta(\beta)) = p_N^{G_2}(\beta, \delta(\beta)) \geqslant p_N^G(\beta, \delta(\beta)) \tag{2.11}$$

where G is any phase (ground state). Lines of coexistence separate the half-plane (δ, T) into regions occupied by single phases. This constitutes the phase diagram in order N.

Suppose that in order N we have found in the phase diagram r phases $G_1, \ldots, G_r$. For any other phase G there are two possibilities:

(i) either at any point (δ, T) there exists a phase G_i such that $p_N^G(\beta, \delta) < p_N^{G_i}(\beta, \delta)$;

or

(ii) there exists a line $\delta_i(\beta)$ of coexistence of G_i and G_{i+1} such that $p_N^G(\beta, \delta_i) = p_N^{G_i}(\beta, \delta_i)$.

What happens if we take some higher order N'? It can be shown that in case (i) there

exists inverse temperature $\beta(N', G)$ such that (i) remains valid in some neighbourhood of $\delta = 0$ for $\beta > \beta(N', G)$. Hence G will not appear in the phase diagram. In case (ii) the addition of new terms to p_N^G may cause G to show up in some region of non-zero width. In general, coexistence lines of order N may split in higher orders and new phases appear.

2.5. *The phase diagram in first order*

In zero order, one compares ground-state energies (2.7). For $\delta > 0$, ground states with $l_o(G) = 1$ dominate. This condition defines $\langle o \rangle$ (o layers only). For $\delta < 0$ one has $l_o(G) = 0$, which defines $<\alpha\beta\rangle$. All other ground states coexist at $\delta = 0$ (cf section 2.2).

In first order we compare quantities

$$p_1^G(\beta, \delta) = \tfrac{3}{2}\delta l_o(G) + (1/\beta) n_1^G(\beta\delta)\, e^{-\beta E_1}.$$

The coefficient n_1^G consists of contributions from lowest-energy excitations (of any ground state). According to the results of section 3.1, these have to be single spin excitations. Using the block technique described in section 3.2, one finds that the lowest energy corresponds to particular excitations of sequences $\alpha\beta o$ or $o\alpha\beta$ (cf table 1) with energy $E_1 = 3J_2$. Hence

$$p_1^G(\beta, \delta) = \tfrac{3}{2}\delta l_o(G) + (1/\beta)[l_{\alpha\beta o}(G) + l_{o\alpha\beta}(G)]\, e^{-3\beta J_2}. \tag{2.12}$$

The above expression is an affine functional in variable δ with a temperature-dependent free term. The phase diagram for such functionals is given by the following algorithm [8]. One constructs the convex envelope for a set $\{3l_o(G)/2,\ (1/\beta)n_1^G(\beta\delta)\ \exp(-3\beta J_2)\}$. Then: (i) maximal extremal points correspond to phases that appear in the zero or first order; (ii) points lying on a maximal extremal edge correspond to phases that are on a coexistence line; (iii) points inside the convex envelope define phases that do not appear in the phase diagram.

In first order there are three maximal extremal points: $(0, 0)$ corresponding to $\langle\alpha\beta\rangle$, $(1/2, (2/3\beta)\exp(-3\beta J_2))$ corresponding to $\langle\alpha\beta o\rangle$ and $(1, 0)$ corresponding to $\langle o\rangle$. The coexistence line between $\langle\alpha\beta\rangle$ and $\langle\alpha\beta 0\rangle$ is given by the solution of

$$0 = p_1^{\langle\alpha\beta\rangle}(\beta, \delta) = p_1^{\langle\alpha\beta o\rangle}(\beta, \delta) = \tfrac{1}{2}\delta + (2/3\beta)\, e^{-3\beta J_2}$$

that is, $\delta = -(4/3\beta)\exp(-3\beta J_2)$. Phases that coexist at this line satisfy the condition

$$-(2/\beta)\, e^{-3\beta J_2}\, l_o(G) + (1/\beta)\, e^{-3\beta J_2}[l_{\alpha\beta o}(G) + l_{o\alpha\beta}(G)] = 0. \tag{2.13}$$

Using structural relations (2.5) we show that

$$\begin{aligned} l_o(G) &= l_{oo}(G) + l_{\alpha o}(G) + l_{\beta o}(G) = l_{oo}(G) + l_{\alpha\beta o}(G) \\ l_o(G) &= l_o(G) + l_{o\alpha}(G) + l_{o\beta}(G) = l_{oo}(G) + l_{o\alpha\beta}(G) \end{aligned} \tag{2.14}$$

since sequences $o\beta$, αo, $o\alpha o$, $o\beta o$ are not allowed. Combining (2.13) with (2.14) we get the condition $l_{oo}(G) = 0$. It defines phases that can be written in the form

$$\langle(\alpha\beta o)^{p_1}(\alpha\beta)^{r_1}(\alpha\beta o)^{p_2}(\alpha\beta)^{r_2}\ldots\rangle \tag{2.15}$$

with $p_i, r_i \geqslant 1$ if $p_1, r_1 \geqslant 1$.

The coexistence line between $\langle\alpha\beta o\rangle$ and $\langle o\rangle$ is $\delta = (4/3\beta)\exp(-3\beta J_2)$. Phases that coexist at this line satisfy the condition $l_{\alpha\beta\alpha}(G) = l_{\beta\alpha\beta}(G) = 0$ and thus have the form

$$\langle(\alpha\beta o)^{p_1} o^{r_1}(\alpha\beta o)^{p_2} o^{r_2}\ldots\rangle. \tag{2.16}$$

2.6. The splitting of coexistence lines: general argument

In orders higher than one we can restrict our discussion to small neighbourhoods of coexistence lines. The form (2.15) and (2.16) of phases that coexist at respective boundaries in order one suggests that we use the general inductive algorithm described in [8]. We recapitulate here briefly the main points of the scheme. The inductive step looks as follows.

Suppose that we have a family of phases that coexist at some boundary $\delta_{N'}(\beta)$ defined in order N'. Let each member of this family have the form

$$\langle A^{p_1}(A^uB)^{r_1}A^{p_2}(A^uB)^{r_2}\rangle \qquad p_i, r_i \geqslant 1 \quad \text{if} \quad p_1, r_1 \geqslant 1 \tag{2.17}$$

where u is fixed (possibly zero). We define the *common core* C as the longest common sub-sequence of $\langle A\rangle$ and $\langle A^uB\rangle$. Obviously C is the longest sequence that appears in all forms (2.17), and it contains A^u as the sub-sequence. In the following we will use sequences $\mu C\nu$, $\mu, \nu = \alpha, \beta, 0$, and their *proper extensions*: M is an extension of M' if it contains M' as a sub-sequence, and M is a proper extension of M' if $l_M(G) = l_{M'}(G)$ for any form (2.17). Let N be the lowest order in which any of the discussed extensions appear in (2.10), and $\delta_N(\beta)$ be the boundary between $\langle A\rangle$ and $\langle A^uB\rangle$ in this order. We make the following assumptions:

(i) For all ground states (2.17), $l_{A^{u+1}}(G)$ and $l_{A^uB}(G)$ can be written as linear combinations of $l_0(G)$ and a constant. Then $l_M(G)$ can also be represented in the same way unless M is an extension of $\mu C\nu$, $\mu, \nu = 0, \alpha, \beta$ (cf [8]).

(ii) If an extension M is not a proper extension of $\mu C\nu$, $\mu, \nu = 0, \alpha, \beta$, then $l_M(G)$ does not appear in (2.10) for all orders $N' \leqslant N$. This assumption is a softer version of condition 1 of [8], and it holds by proposition 2 (section 3.1) and also by the argument at the end of section 3.3.

Next we define

$$a_N(\beta\delta) = \sum_M a_{N,M}(\beta\delta) - \sum_{M'} a_{N,M'-}(\beta\delta) \tag{2.18}$$

where $a_{n,M}$ are defined by (2.10), M is a proper extension of oCo, $\alpha C\alpha$, $\alpha C\beta$, $\beta C\alpha$ or $\beta C\beta$, and M' is a proper extension of $oC\alpha$, $oC\beta$, αCo or βCo. With these assumptions and definitions we have the following result (theorem 2 of [8]).

Theorem. (i) If $a_N(\beta\delta_N(\beta)) > 0$, then no phase (2.17) other than $\langle A\rangle$ and $\langle A^uB\rangle$ appears in the phase diagram.

(ii) If $a_N(\beta\delta_N(\beta)) < 0$, then the boundary between $\langle A\rangle$ and $\langle A^uB\rangle$ is unstable, with the new phase $\langle A^{u+1}B\rangle$ appearing at its locus. In addition:

(a) Phases that coexist at the boundary between $\langle A\rangle$ and $\langle A^{u+1}B\rangle$ satisfy the condition: $l_{BA^uB}(G) = 0$, i.e. $G = \langle A^{p_1}(A^{u+1}B)^{r_1}\ldots\rangle$. Moreover, $l_{A^{u+2}}(G)$ and $l_{A^{u+1}B}(G)$ can be written as linear combinations of $l_0(G)$ and a constant.

(b) Phases that coexist at the boundary between $\langle A^{u+1}B\rangle$ and $\langle A^uB\rangle$ satisfy the condition: $l_{A^{u+2}}(G) = 0$, i.e. $G = \langle (BA^u)^{p_1}(BA^{u+1})^{r_1}\ldots\rangle$. Moreover, $l_{BA^uBA^u}(G)$ and $l_{BA^{u+1}}(G)$ can be written as linear combinations of $l_0(G)$ and a constant.

Remark. The boundary $\delta_N(\beta)$ between phases $\langle A\rangle$ and $\langle A^uB\rangle$ is the solution of (2.11) and hence has the form of the series in $\{\exp(-\beta E_i)\}$. Owing to the results of section 2.5, the free term of this series is zero. Hence the sign of $a_N(\beta\delta_N(\beta))$ for large β is determined by the sign of $a_N(0)$.

2.7. The coexistence line between ⟨αβ⟩ and ⟨αβ0⟩

In this section we apply the results of section 2.6 to the boundary between $\langle\alpha\beta\rangle$ and $\langle\alpha\beta o\rangle$. First let us check that the set of ground states (2.15) indeed satisfies all conditions. Here $A=\alpha\beta$, $B=\alpha\beta o$, $u=0$, $C=\alpha\beta$. Because of (2.5) and (2.14),

$$l_{\alpha\beta 0}(G)=l_0(G) \qquad l_{A^2}(G)=l_{\alpha\beta\alpha\beta}(G)=\tfrac{1}{2}-\tfrac{3}{2}l_0(G).$$

Proper extensions that enter into (2.18) are: $\beta\alpha\beta\alpha$, $\alpha\beta\alpha\beta\alpha$, $\beta\alpha\beta\alpha\beta$, $\alpha\beta\alpha\beta\alpha\beta$ (extensions of $\beta\alpha\beta\alpha$), $o\alpha\beta\alpha$, $o\alpha\beta\alpha\beta$ (extensions of $o\alpha\beta\alpha$), $\beta\alpha\beta o$, $\alpha\beta\alpha\beta o$ (extensions of $\beta\alpha\beta o$) and $o\alpha\beta o$. To find whether the borderline between $\langle\alpha\beta\rangle$ and $\langle\alpha\beta o\rangle$ splits in some higher order N, one has to find a_N. This is done in general terms in section 3.3. We note here that order one may serve as a starting point for the inductive argument.

More generally, let us assume that both sequences A and B entering into (2.17) consist of blocks $\alpha\beta o$ and $\alpha\beta$. Then the common core has one of the forms:

$$C=(\alpha\beta)^{m_1}o(\alpha\beta)^{m_2}o\ldots o(\alpha\beta)^{m_s}\ (s\geqslant 2) \qquad \text{or} \qquad C=(\alpha\beta)^m. \tag{2.19}$$

This sequence can be extended only by $\beta C\alpha$, βCo, $oC\alpha$ and oCo. In section 3.3 we show that the lowest order N in which any of these (or their extensions) appear in the coefficient n_N^G (cf (2.10)) corresponds to the energy

$$E_N=E_{(m_1,m_2,\ldots,m_s)}=5J_2\left(\sum_{i=1}^{s}m_i+s\right) \qquad a_N(0)=-m_1m_2\ldots m_s.$$

Hence for large β part (ii) of the theorem applies. Obviously families of phases that coexist at new borderlines also fall in the pattern described above. Thus we arrive at the inductive scheme, which allows us to describe qualitatively the phase diagram in the neighbourhood of the coexistence line $\langle\alpha\beta\rangle$–$\langle\alpha\beta o\rangle$. It looks as follows (figure 1). In order $E_{(1)}=10J_2$ $(s=1, m=1)$ $\langle(\alpha\beta)^2o\rangle$ appears between $\langle\alpha\beta\rangle$ and $\langle\alpha\beta o\rangle$. Next, $\langle(\alpha\beta)^3o\rangle$ shows up in order $E_{(2)}=15J_2$ $(s=1, m=2)$ between $\langle\alpha\beta\rangle$ and $\langle(\alpha\beta)^2o\rangle$, and $\langle\alpha\beta o(\alpha\beta)^2o\rangle$ separates $\langle\alpha\beta o\rangle$ and $\langle(\alpha\beta)^2o\rangle$ in order $E_{(1,1)}=20J_2$ $(s=2, m_1=m_2=1)$. In general, each coexistence line appearing in some order N bifurcates into two curves in some higher order, as shown schematically in figure 2.

2.8. The coexistence line between ⟨αβo⟩ and ⟨o⟩

It is not hard to check that the set of ground states (2.16) satisfies the conditions of the

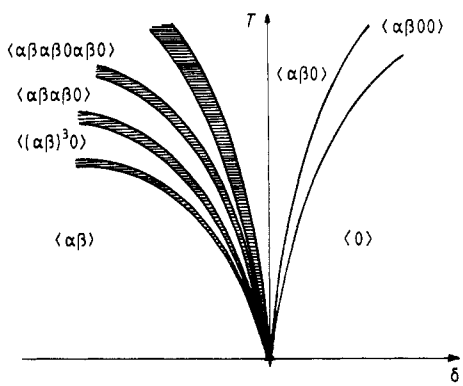

Figure 1. The phase diagram for the model. The shaded region is filled by the bifurcating cascade of phases arranged in the manner shown in figure 2. Phase domains are not to scale.

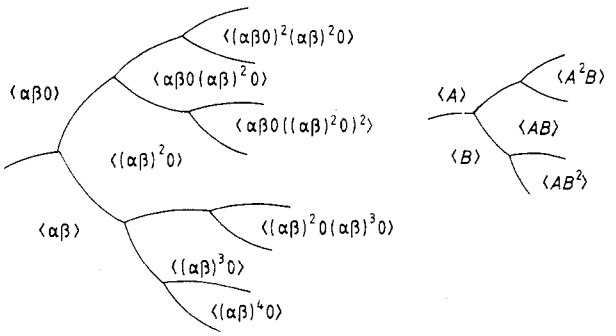

Figure 2. The schematic representation of the bifurcating structure for $\delta < 0$. The scheme is continued in the way shown at the right part of the drawing.

theorem. Here $A = 0, B = \alpha\beta 0, u = 0, C = 0$. Relevant extensions of C are: $\beta o\alpha$, $\alpha\beta o\alpha$, $\beta o\alpha\beta$, $\alpha\beta o\alpha\beta$, βoo, $oo\alpha$, ooo. In section 3.4 we show that the least relevant energy is $E_2 = 6J_2$ and $a_2(0) = -3$ (if $q \neq 4$) or $a_2(0) = -2$ (if $q = 4$). Hence for large β, part (ii) of the theorem applies. The new phase $\langle \alpha\beta oo \rangle$ appears between $\langle \alpha\beta o \rangle$ and $\langle o \rangle$.

The coexistence line $\langle \alpha\beta o \rangle$–$\langle \alpha\beta oo \rangle$. Following the inductive pattern with $A = \alpha\beta o$, $B = 0$, $u = 1$, $C = o\alpha\beta o$ we have to investigate excitations of proper extensions of $oo\alpha\beta oo$, $\beta o\alpha\beta oo$, $oo\alpha\beta o\alpha$ and $\beta o\alpha\beta o\alpha$. This is done in section 3.4. The first relevant order n, in which any of these extensions enters into (2.10), corresponds to $E_n = 29J_2/2$ ($q \neq 4$) or $E_n = 10J_2$ ($q = 4$). Here $a_n(0) = 6$ ($q \neq 4$), $a_n(0) = 9$ ($q = 4$). Hence no new phases appear.

The coexistence line $\langle \alpha\beta oo \rangle$–$\langle o \rangle$. Here $A = o$, $B = o\alpha\beta$, $u = 1$, $C = oo$. In order n with $E_n = 21J_2/2$ we find $a_n(0) = 6$ (cf section 3.4). Hence for large β part (i) of the theorem applies and no new phases appear.

The phase diagram for $\delta > 0$ contains three phases only: the low-temperature $\langle 0 \rangle$ phase, the $\langle \alpha\beta o \rangle$ phase, which occupies the region of small δ, and the intermediate $\langle \alpha\beta oo \rangle$ phase (figure 1).

3. Technical details

3.1. Excitations of a sequence: general remarks

In this and the following sections we will calculate some of the coefficients $a_{n,A}(\beta\delta)$ that appear in front of the structural variables in (2.10). We will restrict our attention to those orders n and sequences A which are important to the preceding discussion.

Let A be of length m, that is it describes the ground-state configuration in m consecutive layers, say $L_0, L_1, \ldots, L_{m-1}$. The coefficient $a_{n,A}(\beta\delta)$ is constructed in the following way. One takes any finite connected set Λ of lattice points such that: (i) if b belongs to Λ or spin at b interacts with any spin in Λ, then b is in one of the layers $L_0, \ldots, L_{m-1}$; (ii) any shorter sequence of layers does not satisfy (i). Here the set is connected if one can pass from one of its points to another by NN or NNN bonds. Next one divides Λ into p possibly overlapping subsets $\Lambda_1, \ldots, \Lambda_p$, $\Lambda = \Lambda_1 \cup \ldots \cup \Lambda_p$. Let

X_i be an excitation differing from G in Λ_i. Any such family of excitations $X_1, \ldots, X_p$ will be referred to as an excitation of the sequence A. If $p > 1$, then we will call it *energetically* disconnected. Finally we require that $E(X_1) + E(X_2) + \ldots + E(X_p) = E_n$. The contribution of the family to $a_{n,A}$ is $(-1)^{p-1}\Gamma \exp\{-\beta\delta[L(X_1) + L(X_2) + \ldots + L(X_p)]\}$, where the factor Γ is positive and equal to one if no two excitations X_i, X_j are identical [13].

In the preceding discussion we needed coefficients $a_{m,A}$ for the lowest order n in which $a_{n,A}$ is non-zero. Hence we face the task of finding the lowest energy excitations of a given sequence A. Such configurations cannot have too many excited spins, which is shown in the following.

Let X be an excitation of A. Points where X differs from the ground-state configuration defined by A are *excited* points. A subset of the lattice (a layer, a triangle, a NNN bond) is excited if it contains excited points. If at most one point in each layer is excited, then such a configuration is called a *linear chain*.

Proposition 1. If X is not a linear chain, then there exists a linear chain Y with the same excited layers and such that $E(X) > E(Y)$.

Proposition 2. Let X and Y be linear chains such that Y is obtained from X by exciting an additional layer. Then $E(Y) > E(X)$.

Proofs of propositions 1 and 2 are based on the straightforward but cumbersome inspection of possibilities and have been omitted.

Proposition 2 first provides the weaker version of condition 1 of [8], which is sufficient for the application of the theorem of section 2.6. Secondly, it allows one to disregard linear chains in which more than two consecutive layers are excited. Hence the minimal energy linear chain has to be built of single-spin and two-NN-spin blocks. The construction of chains out of such blocks is described in the next section.

3.2. *The energy of a linear chain*

Let B be a block consisting of a single spin or two NN spins. The energy E_B of block B is calculated as follows. One takes all NN and NNN bonds that contain points of B as the only excited points. Only two NNN inter-layer bonds are excluded, since they may serve as connections between two neighbouring blocks. Then one calculates for each bond the difference in the interaction value when (i) the block is excited, (ii) the configuration on the block is a ground state. The block energies for various block configurations are given in table 1. One should note that a two-spin block can be energetically discounted, so there are two possible block energies in this case. In table 1 the lower value is given, and the sign (d) means that it corresponds to the disconnected block.

Blocks are connected by the NNN bonds. Energies E_C of bonds are provided in table 2. These bonds also can be energetically disconnected, and both values are given. Finally, blocks located at ends of a chain have the endpoint energy E_E. Values of these are also listed in table 2.

To find the energy of a linear chain, one adds contributions from blocks E_B, bonds E_C and endpoints E_E.

Table 1. Blocks.

Block	Excitation	Energy	Block	Excitation	Energy
$\alpha\beta\alpha$	01210	$5J_2$	$\beta\alpha\beta$	$10(p-1)01$	$5J_2$
01010	$01r10$	$5J_2+3J_1$	10101	$10r01$	$5J_2+3J_1$
$\alpha\beta$o	01212	$3J_2$	o$\alpha\beta$	01012	$3J_2$
01012	$01r12$	$4J_2+3J_1$	01212	$01r12$	$4J_2+3J_1$
βoo	10323	$3J_2+6J_1$	ooα	01032	$3J_2+6J_1$
10123	$10r23$	$4J_2+6J_1$	01232	$01r32$	$4J_2+6J_1$
ooo	01034	$2J_2+6J_1$	βoα	$10r21$	$5J_2+6J_1$
01234 ($q\neq4$)	01434	$2J_2+6J_1$	10121		
	$01r34$	$3J_2+6J_1$			
01230 ($q=4$)	01030	J_2+6J_1			
	$01r30$	$3J_2+6J_1$			
$\alpha\beta\alpha\beta$	$012(p-1)01$	$11J_2-J_1$	$\beta\alpha\beta\alpha$	$10(p-1)210$	$11J_2$ (d)
010101	$012r01$	$11J_2+2J_1$	101010	$10(p-1)r10$	$11J_2+3J_1$ (d)
	$01r(p-1)01$	$11J_2+2J_1$		$10r210$	$11J_2+3J_1$ (d)
	$01r(r+1)01$	$11J_2+4J_1$		$10r(r+1)10$	$11J_2+5J_1$
	$01rs01$	$11J_2+5J_1$		$10rs10$	$11J_2+6J_1$
$\beta\alpha\beta$o	$10(p-1)212$	$9J_2$ (d)	o$\alpha\beta\alpha$	010321	$9J_2$ (d)
101012	$10r212$	$9J_2+3J_1$ (d)	012121	$010r21$	$9J_2+3J_1$ (d)
	$10(p-1)r12$	$10J_2+3J_1$ (d)		$01r321$	$10J_2+3J_1$ (d)
	$10r(r+1)12$	$10J_2+5J_1$ (d)		$01r(r+1)21$	$10J_2+5J_1$ (d)
	$10rs12$	$10J_2+6J_1$		$01rs21$	$10J_2+6J_1$
$\alpha\beta$oo	012323	$6J_2+4J_1$	oo$\alpha\beta$	010123	$6J_2+4J_1$
010123	$01r323$	$\frac{15}{2}J_2+8J_1$	012323	$010r23$	$\frac{15}{2}J_2+8J_1$
	$012r23$	$7J_2+5J_1$		$01r123$	$7J_2+5J_1$
	$01r(r+1)23$	$\frac{17}{2}J_2+7J_1$		$01r(r+1)23$	$\frac{17}{2}J_2+7J_1$
	$01rs23$	$\frac{17}{2}J_2+8J_1$		$01rs23$	$\frac{17}{2}J_2+8J_1$
$\alpha\beta$oα	012321	$8J_2+4J_1$	βo$\alpha\beta$	$10(p-1)012$	$8J_2+4J_1$
010121	$012r21$	$8J_2+5J_1$	101212	$10r012$	$8J_2+5J_1$
	$01r(r+1)21$	$\frac{19}{2}J_2+7J_1$		$10r(r+1)12$	$\frac{19}{2}J_2+7J_1$
	$01rs21$	$\frac{19}{2}J_2+8J_1$		$10rs12$	$\frac{19}{2}J_2+8J_1$
o$\alpha\beta$o	0101323	$7J_2$ (d)	βooα	103432	$\frac{13}{2}J_2+10J_1$
012123	$010r23$	$8J_2+3J_1$ (d)	101232	103132	$5J_1+11J_2$
	$01r323$	$8J_2+3J_1$ (d)		$103r32$	$\frac{13}{2}J_2+11J_1$
	$01r(r+1)23$	$9J_2+5J_1$		$10r032$	$\frac{13}{2}J_2+11J_1$
	$01rs23$	$9J_2+6J_1$		$10(p-1)032$	$\frac{13}{2}J_2+10J_1$
				$10r(r+1)32$	$8J_2+10J_1$
				$10rs32$	$8J_2+11J_1$
βooo	103434	$\frac{9}{2}J_2+10J_1$	oooα	010143	$\frac{9}{2}J_2+10J_1$
101234 ($q\neq4$)	$103r34$	$\frac{11}{2}J_2+11J_1$	012343 ($q\neq4$)	$01r143$	$\frac{11}{2}J_2+10J_1$
	$10r434$	$6J_2+11J_1$		$010r43$	$6J_2+11J_1$
	$10r(r+1)34$	$7J_2+10J_1$		$01r(r+1)43$	$7J_2+10J_1$
	$10rs34$	$7J_2+11J_1$		$01rs43$	$7J_2+11J_1$
101230 ($q=4$)	103030	$3J_2+10J_1$	012303 ($q=4$)	010103	$3J_2+10J_1$
	$10r030$	$\frac{9}{2}J_2+11J_1$		$01r103$	$\frac{9}{2}J_2+11J_1$

Table 1. (*continued*)

Block	Excitation	Energy	Block	Excitation	Energy
oooo	010145	$\frac{7}{2}J_2 + 10J_1$	oooo	$01r(r+1)45$	$6J_2 + 10J_1$
012345	010545	$4J_2 + 11J_1$		$01rs45$	$6J_2 + 11J_1$
($q \neq 4$)					
	014145	$3J_2 + 11J_1$	012301	010101	$3J_2 + 10J_1$
			($q = 4$)		
	014545	$\frac{7}{2}J_2 + 10J_1$		$010r01$	$\frac{7}{2}J_2 + 11J_1$
	$01r145$	$\frac{9}{2}J_2 + 11J_1$		$01r101$	$\frac{7}{2}J_2 + 11J_1$
	$010r45$	$5J_2 + 11J_1$		$01r(r+1)01$	$6J_2 + 10J_1$
	$014r45$	$\frac{9}{2}J_2 + 11J_1$		$01rs01$	$6J_2 + 11J_1$
	$01r45$	$5J_2 + 11J_1$			

3.3. The completion of the inductive argument

In this section we will construct the coefficient $a_N(0)$ (cf (2.18)) for the arbitrary inductive step of section 2.7. The situation is as follows. The common core has the form (2.19) and we have to find the lowest energy excitation of (proper extensions) of $\beta C\alpha$, $\beta C0$, $0C\alpha$ or $0C0$. By preceding sections, we may restrict attention to linear chains built of single-spin and two-NN-spin blocks. For each block we choose the spin configuration with least block energy. As a closer look at table 1 shows, such configurations can always be fitted to one another so that the resulting NNN bond has least energy. We will use the following notation for block and bond configurations with minimal energy (E_B, E_C are calculated for $J_1 = J_2 = 1$):

(i) *Blocks.* a: $\alpha\beta\alpha$, $\beta\alpha\beta$, $E_a = 5$; b: $\alpha\beta$o, o$\alpha\beta$, $E_b = 3$; d: βoα, $E_d = 11$; x^+: $\alpha\beta\alpha\beta$, $E_{x^+} = 10$; x^-: $\beta\alpha\beta\alpha$, $E_{x^-} = 11$ (d); y: $\beta\alpha\beta$o, o$\alpha\beta\alpha$, $E_y = 9$ (d); z: $\alpha\beta$oα, βo$\alpha\beta$, $E_z = 12$; w: o$\alpha\beta$o, $E_w = 7$ (d).

(ii) *Bonds.* α, β: $E_\alpha = E_\beta = 0$; 0: $E_o = -1$ (disconnected).

(iii) *Endpoints.* E^+, E^- denote the energy of the right, left endpoint respectively.

Let n_a be the number of blocks $\alpha\beta\alpha$ and $\beta\alpha\beta$, n_b of blocks $\alpha\beta$o and o$\alpha\beta$, etc. The total energy of a linear chain X is

$$E(X) = 5n_a + 3n_b + 11n_d + 10n_{x^+} + 11n_{x^-} + 9n_y + 12n_z + 7n_w - n_o + E^+ + E^-. \tag{3.1}$$

Table 2. Bonds and endpoints. Excited layers are underlined. Two energy values for bonds correspond to the energetically connected and disconnected NNN bond.

Connection	Excitation	Energy	Endpoint	Excitation	Energy
α, β: $\underline{101}$	$\underline{r0r}$	$0, J_2$	α, β: $\underline{101}$	$\underline{r}01$	$J_2/2$
	$\underline{r0s}$	$J_2/2, J_2$			
o: $\underline{012}$	$\underline{210}$	$0, -J_2$	o: $\underline{012}$	$\underline{2}02$	$-J_2/2$
	$\underline{r01}$	$0, -J_2/2$		$\underline{r}02$	0
	$\underline{21r}$	$0, -J_2/2$			
	$\underline{r1r}$	$-J_2/2, 0$			
	$\underline{r1s}$	$0, 0$			

If X is an excitation of a sequence A, then

$$|A| = 1 + 2(n_a + n_b + n_d) + 3(n_{x^+} + n_{x^-} + n_y + n_z + n_w). \tag{3.2}$$

After solving (3.2) for n_a and substituting into (3.1), the expression for $E(X)$ can be rewritten as

$$2E(X) = 5(|A| - 1) + 2(E^+ + E^-) - 4(n_b + n_y) + 7(n_{x^-} + n_y) - 2n_o + 12n_d + 5n_{x^+} + 9n_z - n_w. \tag{3.3}$$

If $C \neq (\alpha\beta)^m$, then each extension A of $\beta C\alpha$, o$C\alpha$, βCo or oCo consists of segments of the type o$(\alpha\beta)^m$o, and it may contain segments o$(\alpha\beta)^m$, o$(\alpha\beta)^m\alpha$ and the symmetrical ones. If $C = (\alpha\beta)^m$, then A may be any of the above sequences in addition to $(\alpha\beta)^m$, $(\beta\alpha)^m$, $\beta(\alpha\beta)^m$ and $(\alpha\beta)^m\alpha$. Let X_A be the linear chain that inside each segment looks as follows (excited layers are underlined, and each block is in its minimal energy excited configuration):

o$(\alpha\beta)^m$o:	o$\underline{\alpha}\beta\underline{\alpha}\beta\underline{\alpha}\beta \ldots \underline{\alpha}\beta\underline{\alpha}\beta\underline{\alpha}\beta\underline{\alpha}\beta$o, block x^- disconnected;
o$(\alpha\beta)^m$:	o$\underline{\alpha}\beta\underline{\alpha}\beta\underline{\alpha}\beta \ldots \underline{\alpha}\beta\underline{\alpha}\beta\underline{\alpha}\beta\underline{\alpha}\beta$, no two-spin blocks;
$(\alpha\beta)^m$o:	similarly;
o$(\alpha\beta)^m\alpha$:	o$\underline{\alpha}\beta\underline{\alpha}\beta\underline{\alpha}\beta \ldots \underline{\alpha}\beta\underline{\alpha}\beta\underline{\alpha}\beta\underline{\alpha}\alpha$, block x^- disconnected;
$\beta(\alpha\beta)^m$o:	similarly;
$(\alpha\beta)^m$:	$\alpha\underline{\beta}\alpha\underline{\beta}\alpha\underline{\beta} \ldots \alpha\underline{\beta}\alpha\underline{\beta}\alpha\underline{\beta}$;
$(\beta\alpha)^m$:	$\beta\underline{\alpha}\beta\underline{\alpha}\beta\underline{\alpha} \ldots \beta\underline{\alpha}\beta\underline{\alpha}\beta\underline{\alpha}$, block x^- disconnected;
$\beta(\alpha\beta)^m$:	$\beta\underline{\alpha}\beta\underline{\alpha}\beta \ldots \beta\underline{\alpha}\beta\underline{\alpha}\beta$, no two-spin blocks;
$\alpha(\beta\alpha)^m$:	similarly.

The position of the block x^- is arbitrary (it can be replaced by the block y). All α and β bonds are energetically connected, while blocks in adjacent segments are joined by energetically disconnected o bonds.

Proposition 3. X_A is the lowest energy excitation of A.

Proof. First we consider the case $C \neq (\alpha\beta)^m$. Let X be an excitation of A. By the argument of section 3.1, we can assume that X is a linear chain. Let us write $E(X) - E(X_A)$ as the sum over segments:

$$E(X) - E(X_A) = \sum_\sigma \Delta E_\sigma.$$

To ΔE_σ contribute blocks that lie inside the segment, with an exception that blocks d and z and the bond o contribute one half of their energies to each segment containing the o layer. If $0(\alpha\beta)^m$o is not at the end of A, then

$$2\Delta E_{o(\alpha\beta)^m o} = 4(2 - n_b - n_y) + 7(n_{x-} + n_y - 1) + (2 - n_o) + 5n_{x+} + 6n_d + \tfrac{9}{2}n_z \qquad (m \neq 1) \tag{3.4a}$$

$$2\Delta E_{o\alpha\beta o} = -4n_b + (1 - n_w) + (2 - n_o) + 6n_d + \tfrac{9}{2}n_z. \tag{3.4b}$$

For segments at the right end of A we have (similarly for the left end):

$$2\Delta E_{o(\alpha\beta)^m o} = 4(2 - n_b - n_y) + 7(n_{x-} + n_y - 1) + (1 - n_o) + 5n_{x^+} + 6n_d + \tfrac{9}{2}n_z + (E^+ - \tfrac{1}{2}) \qquad (m \neq 1) \tag{3.4c}$$

$$2\Delta E_{o\alpha\beta o} = -4n_b + (1 - n_w) + (1 - n_o) + 5n_{x^+} + 6n_d + \tfrac{9}{2}n_z + (E^+ - \tfrac{1}{2}) \tag{3.4d}$$

$$2\Delta E_{o(\alpha\beta)^m} = 4(1 - n_b - n_y) + 7(n_{x-} + n_y) + (1 - n_o) + 5n_{x^+} + 6n_d + \tfrac{9}{2}n_z + (E^+ - \tfrac{1}{2}) \tag{3.4e}$$

$$2\Delta E_{o(\alpha\beta)^m\alpha} = 4(1 - n_b - n_y) + 7(n_{x-} + n_y - 1) + (1 - n_o) + 5n_{x-} + 6n_d + \tfrac{9}{2}n_z + (E^+ - \tfrac{1}{2}). \tag{3.4f}$$

We want to show that if X differs from X_A in any segment σ, then $\Delta E_\sigma > 0$. First, let us look at $o(\alpha\beta)^m o$ for $m \neq 1$. Then there are no blocks w. Note that since X is spatially connected, either the o layer or one of adjacent α, β layers has to be excited. Hence $n_d + n_z + n_b + n_y = 2$. Furthermore, either the o layer is excited or there is the o bond: $n_o + n_d + n_z = 2$. Finally note that there must be at least one two-spin block, i.e. $n_{x^+} + n_{x-} + n_y + n_z \geq 1$. Simple geometric argument shows that each block x^+ has to be accompanied by two other two-spin blocks. With these conditions taken into account, $\Delta E_\sigma \geq \frac{5}{2}$ if $n_{x^+} + n_z + n_d \neq 0$. Furthermore, $\Delta E_\sigma \geq \frac{7}{2}$ unless $n_y + n_{x-} = 1$. This describes X_A inside $o(\alpha\beta)^m o$. For segments $o(\alpha\beta)^m o$ $(m \neq 1)$ and $o(\alpha\beta)^m\alpha$ at the end of a chain, a similar argument holds with the exception that $n_o + n_d + n_z = 1$, and for $o(\alpha\beta)^m\alpha$ we have $n_b + n_y + n_z + n_d = 1$. Here also $\Delta E_\sigma \geq \frac{5}{2}$.

For $m = 1$ we have $n_{x^+} = n_{x-} = n_y = 0$ and $n_z + n_d + n_o = 2$. If $n_w = 0$, then $n_d = 1 = n_z + n_d$, and $\Delta E_\sigma \geq 2$. Hence $n_w = 1$, which excludes any other block and defines X_A inside $o\alpha\beta o$. Exactly the same argument holds if $o\alpha\beta o$ is at the end of a chain except that $n_o + n_d + n_z = 1$ in this case. Here also $\Delta E_\sigma \geq 2$.

For the segment $o(\alpha\beta)^m$ we have: $n_o + n_d + n_z = 1$, $n_b + n_y + n_z + n_d = 1$. Since two-spin blocks are not obligatory in this case, $\Delta E_\sigma \geq \frac{6}{2}$ unless $n_y = n_z = n_d = n_{x^+} = n_{x-} = 0$ and $n_b = n_o = 1$.

Now let $C = (\alpha\beta)^m$. The above discussion can be applied to extensions with at least one o layer, so is enough to consider sequences with no o layers. Since in this case only n_a, n_{x-} and n_{x^+} are not equal to zero, (3.3) reduces to $2E(X) = \text{const} + 5n_{x^+} + 7n_{x-}$. Next note that: (i) if $A = (\alpha\beta)^m$, then there has to be at least one block x^+; (ii) if $A = (\beta\alpha)^m$, then at least one block $x-$ is needed; (iii) if $A = \alpha(\beta\alpha)^m$ or $\beta(\alpha\beta)^m$, then no two-spin blocks are necessary. This concludes the proof.

Out of common core extensions, only a few need to be considered. Let us take an extension A of $\beta C\alpha$. If A contains but is not equal to $\alpha\beta C\alpha\beta$, then X_A can be obtained from $X_{\alpha\beta C\alpha\beta}$, $X_{\beta C\alpha\beta}$, $X_{\alpha\beta C\alpha}$ or $X_{\beta C\alpha}$ by exciting an additional layer. By proposition 2, $E(X_A)$ is greater than the energy of the corresponding shorter chain. Hence A can be disregarded. A similar argument holds for other extensions of C. The remaining sequences and corresponding minimal excitation energies are as follows. $\alpha\beta C\alpha\beta$: $K + 4$ $(C \neq (\alpha\beta)^m)$, $K + 10 (C = (\alpha\beta)^m)$; $\alpha\beta C\alpha$, $\beta C\alpha\beta$: $K + 5$; $\beta C\alpha$: $K + 6$; βCo, $oC\alpha$: $K + 3$; $\alpha\beta Co$, $oC\alpha\beta$: $K + 2$; oCo: K; $K = 5\sum_{i=1}^{s} m_i + s$. Thus the minimal energy is

$$E_N = E(X_{oCo}) = 5\sum_{i=1}^{s} m_i + s. \tag{3.5}$$

There are $m_1 m_2 \ldots m_s$ different forms of X_{0C0}, corresponding to various locations of blocks x^- or y inside each segment. All forms consist of $2s$ energetically disconnected non-identical components. Hence

$$a_N(0) = (-1)^{2s-1} m_1 m_2 \ldots m_s. \tag{3.6}$$

The above argument provides additional information that extensions of C that are not proper extensions of $\beta C\alpha$, βCo, o$C\alpha$ or oCo can be disregarded. This is the sufficient condition for the application of the theorem of section 2.7 since it allows one to write the coefficient $a_N(\beta\delta)$ in the form (2.18). Otherwise one would have to include in (2.18) extensions that are not proper, and the whole argument could break down [8].

3.4. The form of coefficients a_n for the boundary between $\langle\alpha\beta o\rangle$ and $\langle o\rangle$

In this section we calculate the coefficients a_n that are relevant to the discussion of section 2.8. Since propositions 1 and 2 also hold here, we can use the block technique described in section 3.2. For each case, we write down extensions of a common core and the energy (in units $J_1 = J_2 = 1$) of the corresponding minimal energy linear chain. In several cases the energies for $q \neq 4$ and $q = 4$ are different; the value for $q = 4$ is in parentheses. Excited layers are underlined. Extensions that are not listed may be disregarded (cf the discussion at the end of the preceding section).

The boundary $\langle\alpha\beta o\rangle$–$\langle o\rangle$. The common core is C = o.

o$\underline{\text{o}}$o, 15/2 (6); o$\underline{\text{o}}\alpha$, $\beta\underline{\text{o}}$o, 17/2; $\alpha\underline{\beta}\text{o}\underline{\alpha}\beta$, 6 (d).

The minimal energy is $E_2 = 6$, $a_2(0) = -3$ ($q \neq 4$), $a_2(0) = -2$ ($q = 4$).

The boundary $\langle\alpha\beta oo\rangle$–$\langle o\rangle$. The common core is C = oo.

o$\underline{\text{oo}}$o, 13 (10); o$\underline{\text{o}}$o$\underline{\text{o}}$o, 15 ($q \neq 3, 4$), 29/2 ($q = 3$), 12 ($q = 4$); o$\underline{\text{oo}}\alpha$, $\beta\underline{\text{oo}}$o, 29/2; o$\underline{\text{o}}\text{o}\underline{\alpha}\beta$, $\alpha\underline{\beta}\text{o}\underline{\text{o}}$o, 21/2 (10); $\beta\underline{\text{oo}}\alpha$, 17; $\alpha\underline{\beta}\text{o}\underline{\text{o}}\alpha$, $\beta\underline{\text{o}}\text{o}\underline{\alpha}\beta$, 12.

The minimal energy is $E_n = 21/2$ ($q \neq 4$), for the disconnected excitation of $\alpha\beta$ooo or ooo$\alpha\beta$, and $E_n = 10$ ($q = 4$) for excitations as for $q \neq 4$ and the connected excitation of oooo. Hence $a_n(0) = 6$ ($q \neq 4$), $a_n(0) = 9$ ($q = 4$).

The boundary $\langle\alpha\beta o\rangle$–$\langle\alpha\beta oo\rangle$. The common core is C = 00.

o$\underline{\text{o}}\alpha\underline{\beta}\text{o}\underline{\text{o}}o, o\underline{\text{o}}\alpha\underline{\beta}\text{o}\underline{\text{o}}$o, 37/2; o$\underline{\text{o}}o\alpha\underline{\beta}\text{o}\underline{\text{o}}o, o\underline{\text{o}}\alpha\underline{\beta}o\underline{\text{o}}$o, 19 (35/2); $\beta\underline{\text{o}}\alpha\underline{\beta}\text{o}\underline{\text{o}}o, o\underline{\text{o}}\alpha\underline{\beta}\text{o}\underline{\alpha}$, 21; $\beta\underline{\text{o}}\alpha\underline{\beta}\text{o}\underline{\text{o}}o, o\underline{\text{o}}\alpha\underline{\beta}\text{o}\underline{\alpha}$, 43/2 (21) $\alpha\underline{\beta}\text{o}\underline{\alpha}\beta\underline{\text{o}}o, o\underline{\text{o}}\alpha\underline{\beta}\text{o}\underline{\alpha}\beta$, 29/2 (14); $\beta\underline{\text{o}}\alpha\underline{\beta}\text{o}\underline{\alpha}$, $\beta\underline{\text{o}}\alpha\underline{\beta}\text{o}\underline{\alpha}$, 24; $\alpha\underline{\beta}\text{o}\underline{\alpha}\beta\underline{\text{o}}\alpha$, $\beta\underline{\text{o}}\alpha\underline{\beta}\text{o}\underline{\alpha}\beta$, 17; o$\underline{\text{o}}\alpha\underline{\beta}\text{o}\underline{\text{o}}\alpha$, $\beta\underline{\text{oo}}\alpha\underline{\beta}\text{o}\underline{\text{o}}$, 41/2 (20); o$\underline{\text{oo}}\alpha\underline{\beta}\text{o}\underline{\alpha}$, $\beta\underline{\text{o}}\alpha\underline{\beta}\text{o}\underline{\text{oo}}$, 43/2 (20); $\beta\underline{\text{oo}}\alpha\underline{\beta}\text{o}\underline{\alpha}$, $\beta\underline{\text{o}}\alpha\underline{\beta}\text{o}\underline{\text{o}}\alpha$, 23.

The minimal energy is $E_n = 29/2$ ($q \neq 4$) or $E_n = 14$ ($q = 4$) for the disconnected excitation (NNN pair o$\underline{\alpha}\underline{\beta}$oo and spin $\alpha\underline{\beta}$o) of $\alpha\beta\text{o}\alpha\beta$oo and the corresponding excitation of oo$\alpha\beta\text{o}\alpha\beta$. The contribution is -9, hence $a_n(0) = 18$.

4. Conclusions

In this paper we have shown that the q-state Potts model with the next-nearest-neighbour interaction has an infinite set of phases. This result has been obtained by the LTE

technique, which at best provides for an asymptotic (with $T \to 0$) form of the phase diagram. For systems with an infinite set of ground states it may happen that this approach is valid only for $T = 0$! The reason for this has been briefly discussed in section 2.4: if the phase G is not present in the phase diagram in some order N, then it will not appear in order $N' > N$ only if the inverse temperature exceeds some $\beta(N', G)$. To exclude in order N' all phases that do not show up in order N has to lower the temperature to $\inf\{1/\beta(N', G), G\}$. For systems with an infinite number of ground states this infimum may be zero. The extension of results to non-zero temperatures has in such cases no clear meaning. Therefore other methods should be applied to check the form of the phase diagram. The rigorous analysis of the model remains an open question.

The structure of the phase diagram has the form of the complete Devil's staircase, in contrast to the incomplete Devil's staircase found in the ANNNI and the three-state CC models. The important difference here is the type of interaction anisotropy. In our model each NN bond is ordered and bonds are located isotropically in the lattice. Similar ordering of bonds occurs in the q-state CC model, but in addition bonds are not isotropic in the lattice. In the ANNNI model, the interaction is competitive in one direction and strictly ferromagnetic in the remaining two. The question is whether the anisotropy of the bond location influences the phase diagram structure. The positive answer seems to be supported by the renormalisation group studies of the three-state CC model [3].

Acknowledgments

This work has been supported in part by The Institute of Low Temperatures 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 the condensed phase'.

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