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LOW TEMPERATURE ANALYSIS OF THE AXIAL NEXT-NEAREST NEIGHBOUR ISING MODEL NEAR ITS MULTIPHASE POINT

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CONTENTS

The general, axial next-nearest neighbour Ising (or ANNNI) model in d dimensions consists of $(d-1)$-dimensional layers of spins, $s_i = \pm 1$, with nearest-neighbour ferromagnetic coupling, $J_0 > 0$, within layers but competing ferromagnetic, J_1, and antiferromagnetic, $J_2 < 0$, first- and second-neighbour axial coupling between layers. By systematic low temperature expansions in powers of e^{-2J_0/k_BT}, extended to all orders where necessary, it is shown for $d > 2$ that in the vicinity of a *multiphase* point

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at $T = 0$ and $\kappa = -J_2/J_1 = \frac{1}{2}$ there occurs an infinite sequence of distinct, commensurate modulated phases characterized by wavevectors $q_j = \pi j/(2j+1)a$ for $j = 0, 1, 2, \ldots$. The phase boundaries, $\kappa_j(T)$, and corresponding free energies and interfacial tensions are derived explicitly for low temperatures.

1. Introduction

Many phases of matter are known in which some local property such as magnetization, electric polarization, charge density and chemical composition, exhibits a periodic, spatially modulated structure of wavelength (or wavevector q) which is not related in any direct or obvious way to the underlying structure and interactions of the material but, rather, depends sensitively on such parameters as the temperature and pressure. In this article we address what is, perhaps, the simplest non-trivial statistical mechanical model to exhibit such behaviour, namely, in d spatial dimensions, a spin $\frac{1}{2}$ Ising model with ferromagnetic couplings within $(d-1)$-dimensional layers but competing ferromagnetic and antiferromagnetic interactions between nearest and next-nearest layers along one, unique spatial axis. The abbreviation 'ANNNI model' has been proposed (Fisher & Selke 1980) for this anisotropic, or axial next-nearest neighbour Ising model. Its three-dimensional version on the simple cubic lattice was introduced some years ago by Elliott (1961), who was interested in understanding experimental data on erbium, thulium, and some of their alloys which display 'sinusoidally' modulated magnetic structures. (Other relevant references are given by Selke & Fisher (1979).) The modulated phase in the ferroelectric $NaNO_2$ has also been discussed within the framework of the three-dimensional model by Yamada *et al.* (1963). The ANNNI model on a square lattice has been studied by Hornreich *et al.* (1979) in connection with the existence of a uniaxial Lifshitz point in two-dimensional systems (see also Selke & Fisher 1980*a*, *b*).

We analyse, in this paper, the behaviour of the ANNNI model at low temperatures for $d > 2$ on the basis of a systematic series expansion procedure carried to *all orders* at the vital points. Thence we demonstrate that the model displays an *infinite* number of distinct, spatially modulated, layered magnetic phases which are commensurate with the lattice of spins. The infinity of phases springs from a definite *multiphase point* at $T = 0$, corresponding to a parameter value, $\kappa = \kappa_0$, for which the ground state becomes infinitely degenerate.

There is another model, namely a one-dimensional classical chain of anharmonically coupled particles (Frank & van der Merwe 1949), which, as demonstrated by Aubry (1978), also exhibits an infinite number of commensurate phases as a parameter, κ, is varied: owing to its one-dimensional character, however, no distinct thermodynamic phases survive at non-zero temperature in this model. However, at $T = 0$, the wavevector $\bar{q}(\kappa)$ specifying the periodicity 'locks in' at each rational fraction of the fundamental reciprocal lattice vector: Aubry (1978) identified the corresponding, continuous graph of $\bar{q}(\kappa)$ as a 'devil's staircase' (Mandelbrot 1977). A devil's staircase behaviour has also been suggested as a possibility for ANNNI models by von Boehm & Bak (1979) on the basis of mean-field calculations (which effectively reduce the problem to the class of classical one-dimensional ground state, fluctuationless models studied generally by Aubry). These authors were motivated by the numerous spatially modulated magnetic phases observed in CeSb. However, on the basis of further calculations which made allowance for thermal fluctuations in the magnetic layers, Bak & von Boehm (1980) modified their conclusions and felt able to demonstrate the existence, at low tempera-

tures, of only relatively few commensurate phases. An interesting more recent phenomenological analysis of the ANNNI model, also directed toward gaining a theoretical understanding of CeSb, has been presented by Villain & Gordon (1980).

While our systematic low temperature analysis of the ANNNI model demonstrates (for $d > 2$) an infinite number of phases, the wavevector, $\bar{q}(T, \kappa)$, at low temperatures locks in only at certain rational fractions of the reciprocal lattice, specifically at $\bar{q} = \pi j/(2j+1)a$ for all integral j, where a is the interlayer lattice spacing. (Various phases found by Bak & von Boehm (1979, 1980) are definitely excluded at low temperatures.) However, as a function of T or κ, the extent of the jth phase decreases exponentially with j as the limiting phase boundary, $\kappa_\infty(T)$, of the so-called (2, 2) antiphase state is approached (see below). The graph of $\bar{q}$ then displays quasi-continuous behaviour at the limiting point (see figure 6) which might be termed a 'devil's step'. (This feature appears to disagree with the conclusions reached by Villain & Gordon (1980).)

It is, of course, worth while to discuss the relevance of such peculiar behaviour to observations on real systems (see, for example, Aubry 1978; Bak & von Boehm 1980; Villain & Gordon 1980).† Here, however, we present only the mathematical analysis of the model. A preliminary mention (Selke & Fisher 1980*a*), and a summary of the main results and an outline of the theoretical approach (Fisher & Selke 1980) have appeared. In the following section the class of ANNNI models is specified precisely, and our terminology and notation are explained. The ground states are discussed in §3, and the set of first excited states is analysed in §4. The phase boundary and interfacial tensions between the ferromagnetic and (3, 3) antiphase state are obtained to higher order in §§5 and 6. The basic analysis of the phase diagram between the limiting (3, 3) and (2, 2) antiphase states is broached in §7. This proceeds through the introduction in §8 of an infinite set of *standard structural variables*, l_ν, which specify all allowable ground states and permit the construction of low temperature expansions for the free energies of all possible modulated phases (§§9, 10, 11). Finally, the full sequence of stable phases can be determined (§12) by an inductive argument. The corresponding phase boundaries, interfacial tensions, and wavevector dependencies are obtained in §§13 and 14. Some crucial but more detailed considerations concerning the expansion to general order are presented in the Appendix.

2. The model, terminology, and notation

The Hamiltonian of the axial next-nearest neighbour spin $\frac{1}{2}$ Ising model on a lattice constructed of equivalent $(d-1)$-dimensional layers (the ANNNI model) may be written explicitly as

$$\mathscr{H} = -\tfrac{1}{2} \sum_{i,j,j'} (J_0 s_{i,j} s_{i,j'} + J_1 s_{i,j} s_{i\pm1,j} + J_2 s_{i,j} s_{i\pm2,j}), \tag{2.1}$$

where $s_{i,j}$ is the spin in the layer i at the site (i, j) which interacts ferromagnetically, $J_0 > 0$, with its $q_\perp$ nearest neighbours, $s_{i,j'}$ in the layer i. We suppose the layers are stacked 'vertically', so that the coordination number of the full d-dimensional lattice is given by $q = q_\perp + 2$. The coupling $J_1 > 0$ between $s_{i,j}$ and its two nearest-neighbour spins $s_{i\pm1,j}$ in adjacent layers

† It is worth noting that the sequence of wavevectors originally claimed for CeSb by Rossat-Mignod *et al.* (1977), namely $\bar{q} = \pi j/(2j-1)a$, follows from our results for an ANNNI model with *anti*ferromagnetic interactions between *both* n.n. and n.n.n. layers, merely by inverting the sense of the spins in alternate layers, as discussed by Villain & Gordon (1980).

(at a lattice spacing $a \equiv 1$), is taken to be ferromagnetic, while the corresponding coupling between $s_{i,j}$ and its two second neighbours along the z-axis at spacing $2a$ (the axial second neighbours) is taken to be antiferromagnetic, $J_2 < 0$, and so competes with the nearest-neighbour axial coupling.

A finite ANNNI model will be taken as composed of L layers of M spins (coupled with periodic boundary conditions), so that the total number of spins will be $N = LM$.

At zero temperature, $T = 0$, the properties of the model can easily be found exactly (see §3). The structure of any *ground state* is specified by the spin orientation 'up' or 'down' of each layer: because $J_0 > 0$ all spins in a given layer must point the same way in any ground state. The ground state structure can thus be described by *structural sequences* denoted by μ or ν, specifying sequences of *bands* where a *band* is a set of 1, 2, 3, ... adjacent, identically oriented layers, terminated at both ends by oppositely oriented layers. Since there is no external magnetic field term in (2.1) the energy of any configuration is invariant to a total reversal of all spins: thus it is unnecessary to specify whether a given band, or overturned spin in a band, is oriented 'up' or 'down'. The *length*, $m(\mu)$, *of a band-sequence* is defined as the number of bands in the sequence: for example, $\mu_1 = 32331$ is a 5-band sequence. The same overall ground state structure can be described by specifying different band-sequences of different lengths, but certain specifications determine unique overall structures. Thus the structure with one band of length L is just the fully ferromagnetic ground state (where, since we restrict all considerations to zero external magnetic field, the twofold 'up–down' degeneracy may be ignored). A band-sequence μ without the first and the last band specified will be called the *core* or the *structural core* and will be denoted by $\tilde{\mu}$: for example, $\tilde{\mu} = 233$ is the core of the 5-band example given above. If the ground state structure is periodic, it can be characterized by a wavelength λ or a wavenumber $\bar{q} = 2\pi/\lambda$ (the convention of unit lattice spacing a being used).

The ANNNI model will be studied at non-zero temperatures in the framework of a systematic low temperature expansion. The parameters of the expansion will be the elementary Boltzmann factors

$$w = \mathrm{e}^{-2K_0} \quad \text{and} \quad x = \mathrm{e}^{-2K_1}, \tag{2.2}$$

where for $i = 0, 1, 2$ the reduced exchange integrals are

$$K_i = J_i/k_{\mathrm{B}}T, \tag{2.3}$$

in which k_{B} is Boltzmann's constant. The expansion will focus particularly on the region of the infinitely degenerate ground state which occurs when the basic field parameter

$$\kappa = -J_2/J_1 = \tfrac{1}{2} + \delta > 0 \tag{2.4}$$

takes the special value $\kappa = \frac{1}{2}$ (corresponding to $\delta = 0$). Then the thermodynamic state of the whole system is determined by w, x, and δ. Our aim will be to describe as completely as possible the phase diagram of the model in the (T, κ)-plane (at fixed J_0 and J_1) for low temperatures. (For intermediate and high temperatures, see Selke & Fisher (1979, 1980*a*) and references therein and the references to Bak, von Boehm, Villain and Gordon cited in the Introduction.)

In constructing low temperature expansions about a given ground state, it is necessary to determine the energy, ΔE_ω, contributed to the ground state by a particular type of spin, to find the corresponding excitation energy ϵ_ω associated with 'overturning' such a spin, and,

more generally, to obtain the excitation energies associated with overturning a *configuration* of neighbouring spins of character ω. In addition, the number, N_ω, of realizations of a configuration, ω, in a given ground state must be calculated. The energies ΔE_ω, ϵ_ω, and the *configurational counts*, N_ω, can, as we will show, be determined uniquely if sufficiently many *structural variables*, $l_\mu \equiv [\mu]$, for low-order band-sequences μ are known for the ground states in question. This crucial fact is simply a consequence of the finite range of the interactions in the ANNNI model Hamiltonian (2.1). As regards single spins, it thereby suffices to consider only the following configurations, in which a caret denotes the spin in question, while the plus and minus signs indicate the relative orientations ('up' or 'down') of the successive layers neighbouring the spin:

bulk spin:	$+ + \hat{+} + +$	o
near-edge spin:	$+ + \hat{+} + -$	π
centre spin:	$- + \hat{+} + -$	ρ
edge spin:	$+ + \hat{+} - -$	σ
two-band spin:	$- + \hat{+} - -$	τ.

(2.5)

The labels o, π, and ρ, σ and τ will be used for brevity in the calculations. The latter play a particular role since it transpires that for $T > 0$ only bands of width 2 or 3 consecutive aligned layers (2-bands and 3-bands) are of significance in the principal expansions.

It is easy to see that the structural variables $l_\mu \equiv [\mu]$ cannot all be varied independently. Specifically, we will establish that they obey a set of definite linear *structural relations* (see §7). Using these, we may define a reduced set of *standard structural variables*, $l_\nu \equiv [\nu]$; through these we can define a series of *structural spaces*, $\mathscr{L}_n$, of order n within which all possible (relevant) ground states will be represented (see §10 and Appendix). Important general structures are those generated from a structural sequence μ by periodic repetition to obtain a full infinite lattice structure: such periodic structures will be denoted by $\langle\mu\rangle$ (Fisher & Selke 1980).

By calculating, for all possible ground states, the free energies, which turn out to be linear functions of the standard structural variables l_μ with *structural coefficients* $a_\mu(w, x; \delta)$, we can determine the thermodynamic state realized for given (w, x, δ) by minimizing the free energy: this yields a linear programming problem on the $\mathscr{L}_n$ which can be solved recursively. The details of this program and necessary further terminology are explained in the following sections.

3. Ground states

Clearly, in the ground state at $T = 0$ the spins in each layer are ordered ferromagnetically, since $J_0 > 0$. Then the orientations of all spins, and thence the configuration of the whole lattice, are specified by a set of band-sequences. To describe all possible configurations (from which we will determine the ground states for various $J_1 > 0$ and $J_2 < 0$), we first introduce the structural variables, l_k, by

$$L_k = l_k L, \quad k = 1, 2, 3, \ldots, \tag{3.1}$$

where L_k is the number of k-layer bands, or k-bands (sequences of k identically oriented adjacent layers terminated by oppositely oriented layers) in a given ground state structure. Clearly we must then have

$$\sum_{k \geqslant 1} k L_k = L \quad \text{and} \quad \sum_{k \geqslant 1} k l_k = 1. \tag{3.2}$$

We first show that $L_1 \equiv 0$ in any ground state with $J_1 > 0$ and $J_2 = -(\frac{1}{2}+\delta)J_1 < 0$ with $|\delta| < \frac{1}{2}$. (Actually, this result is true for all $J_2 < 0$, but, because we are here interested primarily in small values of δ, we may present a simpler proof.) Now any one-layer band (say of 'up' spins) can be obtained by flipping one layer of 'down' spins surrounded by adjacent layers of down spins. The second neighbour layers may be either (i) both up layers, or (ii) one up and one down layer, or (iii) both down layers. The energy per spin associated with such a flip is then easily found from (2.1) to be

$$\begin{aligned} \epsilon &= 2J_1(3+2\delta) \quad \text{for (i)}, \\ &= 4J_1 \quad\quad\quad\quad \text{for (ii)}, \\ &= 2J_1(1-2\delta) \quad \text{for (iii)}. \end{aligned} \tag{3.3}$$

Hence for $-\frac{3}{2} < \delta < \frac{1}{2}$ we have $\epsilon > 0$, and the flipped state always has the larger energy. Thus any structure with a one-band layer cannot be a ground state. Henceforth, we may thus assume $L_1 = l_1 = 0$: the only possible ground states consist of multilayer bands.

To determine the energy of a given configuration of ferromagnetic layers we recall the five distinct types of spin (representing whole layers) defined in (2.5). The numbers of these various types of spin in a given configuration of multilayer bands, $\{L_k\}$ or $\{l_k\}$, are

$$N_0 = N \sum_{k\geqslant 5} (k-4)\, l_k, \tag{3.4}$$

$$N_\pi = N \sum_{k\geqslant 4} 2l_k, \quad N_\rho = Nl_3, \tag{3.5}$$

$$N_\sigma = N \sum_{k\geqslant 3} 2l_k, \quad N_\tau = 2Nl_2. \tag{3.6}$$

These identities are precise only for $L \gg 1$, but become exact in the thermodynamic limit. (For finite L, boundary effects should be considered, but they are of no significance when $L \to \infty$.) By considering the distribution of 'right' (low energy) and 'wrong' (high energy) bonds for the five types of spin layer, one finds that, in addition to the in-layer contribution per spin of $-\frac{1}{2}q_\perp J_0$, the following contributions to the ground state (per spin):

$$\Delta E_0 = -\tfrac{1}{2}(1-2\delta)J_1, \tag{3.7}$$

$$\Delta E_\pi = -J_1, \quad \Delta E_\rho = -\tfrac{1}{2}(3+2\delta)J_1, \tag{3.8}$$

$$\Delta E_\sigma = 0, \quad \Delta E_\tau = -\tfrac{1}{2}(1+2\delta)J_1. \tag{3.9}$$

By combining these results the total ground state energy per spin can be written

$$E_0\{l_k\} = -\tfrac{1}{2}q_\perp J_0 - \tfrac{1}{2}J_1 - J_1\,\delta[2l_2 + l_3 - \sum_{k\geqslant 5}(k-4)\,l_k], \tag{3.10}$$

which is subject to the constraints

$$\sum_{k\geqslant 2}^{L} k l_k = 1 \quad \text{and} \quad l_k \geqslant 0 \quad (\text{all } k). \tag{3.11}$$

Determining the true ground state is now a trivial linear programming problem. For $\delta < 0$, the square-bracketed expression multiplying δ must be as negative as possible. Clearly this occurs when $L_\infty = 1$ and $l_k = 0$ for $k < \infty$. Hence the ground state is the ferromagnetic state with

$$E_{0\langle\infty\rangle} = -\tfrac{1}{2}q_\perp J_0 - \tfrac{1}{2}J_1 + \delta J_1 \quad (\delta \leqslant 0), \tag{3.12}$$

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where the notation $\langle\infty\rangle$ denotes the ∞-band fully ferromagnetic state. Conversely, for $\delta > 0$ the square bracket has to be as positive as possible. This yields $l_2 = \frac{1}{2}$, and $l_j = 0$ for $j \geqslant 3$. The ground state must clearly then be the so-called (2, 2) antiphase state of alternating 'two-up', 'two-down' bands (Selke & Fisher 1979, 1980*a*), which we denote as $\langle 2\rangle$ in accordance with the convention mentioned in the previous section. The corresponding energy is

$$E_{0\langle 2\rangle} = -\tfrac{1}{2}q_\perp J_0 - \tfrac{1}{2}J_1 - \delta J_1 \quad (\delta \geqslant 0). \tag{3.13}$$

Finally, *at* $\delta = 0$ the ground state is evidently infinitely degenerate with any sequence of 2-bands, 3-bands, ..., j-bands, ... having the same energy

$$E_{00} = -\tfrac{1}{2}q_\perp J_0 - \tfrac{1}{2}J_1. \tag{3.14}$$

Note, however, that the entropy per spin is zero for $d \geqslant 2$, since the degeneracy is obviously smaller than 2^L (the number of all possible structures $\{l_k\}$ with allowance made for nonzero l_1) in all ground states.

4. First excited states

To analyse the ANNNI model at nonzero temperatures in the interesting region near $\kappa = \frac{1}{2}$ or $\delta = 0$ we construct low temperature expansions for the free energy from all the possible degenerate ground states at $\kappa = \frac{1}{2}$ specified by $\{l_k\}$ with $l_1 = 0$. For the first excited states one needs only the five types of elementary spin flips corresponding to the five types of configuration $\lambda = \mathrm{o}, \pi, \rho, \sigma$ and τ displayed in (2.5). It is straightforward to check that one has

$$\epsilon_\lambda = 2q_\perp J_0 - 4\Delta E_\lambda, \tag{4.1}$$

where the ΔE_λ are just the ground state configurations listed in (3.7)–(3.9). In terms of the variables w and x, defined in (2.2), the corresponding Boltzmann factors, or *weights*, $\mathrm{e}^{-\epsilon_\lambda/k_\mathrm{B}T}$, are thus simply

$$w^{q_\perp}x^{1-2\delta}, \quad w^{q_\perp}x^2, \quad w^{q_\perp}x^{3+2\delta}, \quad w^{q_\perp}, \quad w^{q_\perp}x^{1+2\delta}, \tag{4.2}$$

respectively (Domb 1960).

The partition function expansion about a given ground state structure can be written

$$Z_N\{l_k\} = \exp\left[-NE_0\{l_k\}/k_\mathrm{B}T\right]\{1 + \sum_{n=1} \Delta Z_N^{(n)}\}, \tag{4.3}$$

where the superscript (n) denotes the total contributions from n individual overturned spins or spin flips. It is clear, by using the configurational counts N_λ given in (3.4)–(3.6), that

$$\begin{aligned}\Delta Z_N^{(1)}/N &= \sum_\lambda (N_\lambda/N)\exp\left(-\epsilon_\lambda/k_\mathrm{B}T\right),\\ &= w^{q_\perp}[x^{1-2\delta}\sum_{k\geqslant 5}(k-4)\,l_k + 2x^2\sum_{k\geqslant 4} l_k\\ &\qquad + x^{3+2\delta}l_3 + 2\sum_{k\geqslant 3} l_k + 2x^{1+2\delta}l_2],\end{aligned} \tag{4.4}$$

where we have also used (4.2). More generally as $w \to 0$ (or, equivalently, $T \to 0$ at fixed J_0, J_1, and κ) one sees that $Z_N^{(n)}$ is of order $w^{p_0(n)}$, where $p_0(n)$ is the smallest bond-perimeter encompassing a cluster of n spins on a $(d-1)$-dimensional lattice layer. Explicitly one always has

$$p_0(1) = q_\perp \equiv q - 2, \quad p_0(2) = 2q_\perp - 2, \quad p_0(3) = 3q_\perp - 4.$$

For larger n and $d > 2$ one finds that $p_0(n)$ increases with n as $n^{(d-2)/(d-1)}$ (as seen by considering a layer cluster of diameter of order $n^{1/(d-1)}$). Consequently, we can expect to generate from

(4.3) a convergent series for the free energy in powers of w: this is the standard approach for generating low temperature expansions in Ising models (see, for example, Domb 1960). The same result is used in the Peierls–Griffiths proof of the existence of a stable low temperature phase and associated phase transition. Note, however, that the construction fails for $d = 2$, or one-dimensional layers, since one then has $p_0(n) = 2$ for all $n \geqslant 1$, and the resulting series do *not* converge. Hence our considerations are restricted to $d > 2$.

Given these facts, the reduced free energy per spin may now be expanded in leading order as

$$f\{l_k\} = \frac{-F_N\{l_k\}}{Nk_B T} = \frac{-E_0}{k_B T} + \frac{\Delta Z_N^{(1)}}{N} + O(w^{2q_\perp - 2}), \tag{4.5}$$

or, explicitly from (4.4) on eliminating l_3 by using (3.11), as

$$f = \tfrac{1}{2}q_\perp K_0 + \tfrac{1}{2}K_1 + \tfrac{1}{3}K_1\delta + \tfrac{1}{3}(2 + x^{3+2\delta})\, w^{q_\perp} + a_2(\delta)\, l_2 + \sum_{k \geqslant 4} a_k(\delta)\, k l_k, \tag{4.6}$$

with the *structural coefficients* given by

$$a_2(\delta) = \tfrac{4}{3}K_1\delta - \tfrac{2}{3}(2 - 3x^{1+2\delta} + x^{3+2\delta})\, w^{q_\perp} + O(w^{2q_\perp - 2}), \tag{4.7}$$

and, for $k \geqslant 4$,

$$k a_k(\delta) = -\tfrac{4}{3}K_1\delta(k-3) - [\tfrac{2}{3}(k-3) - (k-4)\, x^{1-2\delta} - 2x^2 + \tfrac{1}{3}kx^{3+2\delta}]\, w^{q_\perp} + O(w^{2q_\perp - 2}). \tag{4.8}$$

To obtain the correct free energy to leading order we need to maximize $f\{l_2; l_4, l_5, \ldots\}$ at fixed δ subject only to $l_k \geqslant 0$ and $\Sigma_{k \geqslant 4} k l_k \leqslant 1 - 2l_2$. The possible structures of the phases at non-zero T will then be restricted by the optimizing values found for the l_k.

Now note that $a_2(\delta)$ is positive only for $\delta > \delta_1^{(1)}(T)$, where $\delta_1^{(1)}$ is defined by

$$a_2(x, w; \delta_1^{(1)}) = 0, \tag{4.9}$$

the superscript serving to indicate that, at this stage, only single spin excitations have been considered. Conversely, for $k \geqslant 4$ one sees that $a_k(\delta)$ is positive only for $\delta < \delta_{-k}(T)$, where

$$a_k(x, w; \delta_{-k}) = 0 \quad (k \geqslant 4). \tag{4.10}$$

Solving these equations to leading order yields

$$K_1\delta_1^{(1)} = w^{q_\perp}(1-x)^2(1 + \tfrac{1}{2}x) + O(w^{2q_\perp - 2}), \tag{4.11}$$

while, for $k \geqslant 4$, one finds

$$K_1\delta_{-k} = -\tfrac{1}{2}w^{q_\perp}(1-x)^2[1 + \tfrac{1}{2}kx/(k-3)] + O(w^{2q_\perp - 2}), \tag{4.12}$$

$$a_k(\delta) = \tfrac{4}{3}K_1[1 - (3/k)]\,(\delta_{-k} - \delta)\,[1 + O(w^{q_\perp - 2})]. \tag{4.13}$$

From these last two results it follows that for $\delta < 0$ the inclusion of any band of width $k \geqslant 4$ can only decrease f relative to the inclusion of a wider band with $k' > k$. Consequently, for $\delta < \delta_{-\infty}(T)$ the fully ferromagnetic state, $\langle\infty\rangle$, is stable against the intercalation of any layers of width $k \geqslant 4$. We conclude that (at least) three regions of stable phases originate at $T = 0$, $\delta = 0$: (*a*) for $\delta < \delta_{-\infty}$, a ferro-phase with $L_\infty = 1$ and $l_k = 0$ (all $k < \infty$); (*b*) for $\delta_{-\infty} < \delta < \delta_1^{(1)}$, a phase in which $l_2 = 0$ and $l_k = 0$ for $k \geqslant 4$, so that $l_3 = \frac{1}{3}$ which clearly specifies the (3, 3) antiphase state which, in accord with our conventions, we denote by $\langle 3\rangle$; and (*c*) for $\delta > \delta_1^{(1)}$, a phase with $l_2 = \frac{1}{2}$ and $l_k = 0$ for all $k \neq 2$, which again specifies the (2, 2) antiphase state $\langle 2\rangle$.

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In the next two sections we examine the phase boundary $\langle\infty\rangle\langle 3\rangle$, which we will call $\delta_0(T)$ in place of $\delta_{-\infty}(T)$, in more detail and also digress further to examine some additional features of the ferro-phase. However, since the arguments so far presented establish that no phases beyond $\langle\infty\rangle$ and $\langle 3\rangle$ can appear in the vicinity of $\delta = \delta_{-\infty}(T) \equiv \delta_0(T)$ (at least at low enough temperatures), the next two sections are not essential to the logical development of the proof that, in fact, an infinite number of commensurate phases spring from the point $T = 0$, $\delta = 0$.

5. Higher-order analysis of ferro-(3, 3) boundary

The calculation of f to order $n = 3$ (three spin-flips) is made later in generality. A direct two-flip calculation of $f_{\langle 3\rangle}$ is not hard and yields

$$f_{\langle 3\rangle} = \tfrac{1}{2}q_\perp K_0 + \tfrac{1}{2}K_1 + \tfrac{1}{3}K_1\delta + \tfrac{2}{3}w^{q_\perp}(1+\tfrac{1}{2}x^{3+2\delta}) + \tfrac{1}{3}q_\perp w^{2q_\perp-2}(1+\tfrac{1}{2}x^{6+4\delta}) - \tfrac{1}{3}w^{2q_\perp}[(q+1) - 3x^{1+2\delta} - 3x^2 + 4x^{3+2\delta} + \tfrac{1}{2}(q-1)x^{6+4\delta}] + O(w^{3q_\perp-4}), \quad (5.1)$$

where we have used $q_\perp = q-2$. The calculation of $f_{\langle\infty\rangle}$ involves only spins of the type o and is a standard calculation. To second order one finds

$$f_{\langle\infty\rangle} = \tfrac{1}{2}q_\perp K_0 + \tfrac{1}{2}K_1 - K_1\delta + w^{q_\perp}x^{1-2\delta} + \tfrac{1}{2}q_\perp w^{2q_\perp-2}x^{2-4\delta} + w^{2q_\perp}[x^{-4\delta} - \tfrac{1}{2}(q+3)x^{2-4\delta} + x^{3-2\delta}] + O(w^{3q_\perp-4}). \quad (5.2)$$

Equating (5.1) and (5.2) gives a relation for the $\langle\infty\rangle\langle 3\rangle$ phase boundary, which may be solved recursively to yield

$$K_1\delta_0 = -\tfrac{1}{2}w^{q_\perp}(1-x)^2(1+\tfrac{1}{2}x) - \tfrac{1}{4}q_\perp w^{2q_\perp-2}(1-x^2)^2(1+\tfrac{1}{2}x^2) + \tfrac{1}{4}w^{2q_\perp}[q+4-9x-\tfrac{3}{2}(q-1)x^2+5x^3+\tfrac{1}{2}(q-3)x^6] + O(w^{3q_\perp-4}). \quad (5.3)$$

We may also calculate the phase boundary $\langle\infty\rangle\langle 3\rangle$ without expanding this way, by solving numerically the implicit equation for δ_0, which follows from equating (5.1) and (5.2). The result is shown in figure 1, where we have also included the solutions for the analogous expressions to third order of the low temperature expansions. In the latter case, $f_{\langle 3\rangle}$ has been obtained from table 3 (p. 18), while $f_{\langle\infty\rangle}$ can be obtained to this order in a straightforward calculation. Note that the numerical results are for the simple cubic lattice with $J_0 = J_1$. In this case, we can compare the low temperature expansion results with the previous Monte Carlo calculations (Selke & Fisher 1979, 1980*a*) and with the mean-field calculations (Bak & von Boehm 1979, 1980). For example, at $\delta = -0.05$ (or $\kappa = 0.45$) one finds quite good agreement: the low temperature expansion gives a transition temperature of $2.8J_1/k_B$ just as does the Monte Carlo calculation; the mean field result is about $3.2J_1/k_B$. However, for larger negative values of δ the Monte Carlo transition temperatures lie below the values of the low temperature expansion, which might well indicate the instability of the $\langle 3\rangle$ phase in that part of the phase diagram (see below). Close to $\delta = 0$, the Monte Carlo simulation becomes unreliable and the present series expansion results will be accurate.

To establish the order of the phase boundary between $\langle\infty\rangle$ and $\langle 3\rangle$ we analyse the interfacial or surface tension. To define the surface tension, consider a mixed phase structure $\langle\infty\rangle{:}\langle 3\rangle$, consisting of a sequence of j_1 up layers followed by $j_2\Lambda_2$ ($\Lambda_2 = 3$) layers of the (3, 3) anti-phase type, i.e. three down layers alternating with three up layers. One can introduce the phase fractions $\theta_1 = j_1/L$ and $\theta_2 = \Lambda_2 j_2/L$ where, clearly, $\theta_1 + \theta_2 = 1$. As always, we assume periodic boundary conditions. Thus the reduced free energy per spin of $\langle\infty\rangle{:}\langle 3\rangle$ may be written

$$f_{\langle\infty\rangle:\langle 3\rangle} = \theta_1 f_{\langle\infty\rangle} + \theta_2 f_{\langle 3\rangle} + 2\Sigma_0/k_B T, \quad (5.4)$$

where $\Sigma_0(x, w, \delta)$ with $\delta = \delta_0(T)$ represents the surface tension on the phase boundary $\langle\infty\rangle\langle 3\rangle$ (for an interface normal to the anisotropy axis). Now $f_{\langle\infty\rangle:\langle 3\rangle}$ can be calculated without difficulty for single spin flips, appropriate account being taken of the configurations near the phase boundary. Then, on using (5.1)–(5.3) and comparing with (5.4), one obtains to the leading order

$$\Sigma_0/k_B T \approx \tfrac{1}{2} w^q \perp x(1-x)^2. \tag{5.5}$$

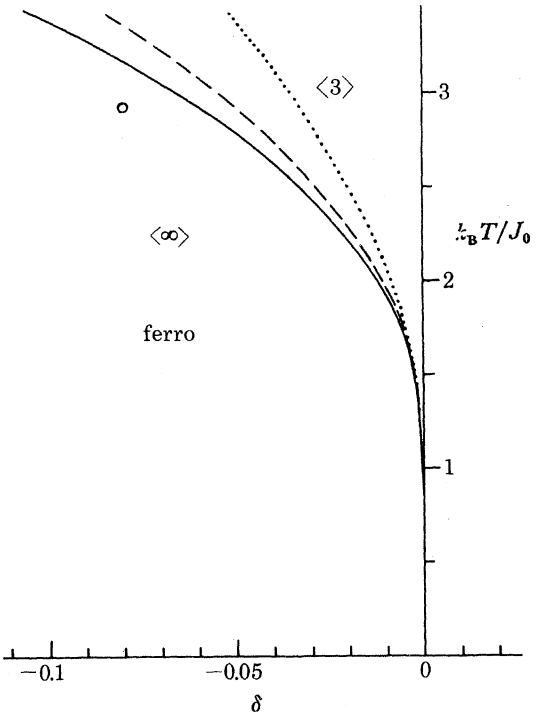

FIGURE 1. The ferromagnetic-to-(3, 3) antiphase ($\langle\infty\rangle\langle 3\rangle$) boundary in third order (solid curve), second order (broken curve), and first order (dotted curve) of the low temperature expansions for the simple cubic lattice with $J_0 = J_1$. The Monte Carlo estimate shown for $\delta \approx -0.08$ (open circle) suggests that the third-order series are inadequately converged for $|\delta| \gtrsim 0.05$.

For non-zero temperatures, and the whole physical range $0 < x < 1$, the surface tension is evidently positive for small w (i.e. low temperatures). We conclude that the transition between the ferromagnetic, $\langle\infty\rangle$, phase and the (3, 3), or $\langle 3\rangle$, phase is of *first order*. A similar conclusion follows by comparing the discontinuity in energy or entropy across the phase boundary $\delta_0(T)$.

It is worth while to make a few observations regarding the phase transition from the ferromagnetic phase at higher temperatures. From the phase diagram of the ANNNI model determined numerically for the simple cubic lattice with $J_0 = J_1$ by Monte Carlo and mean-field techniques (Selke & Fisher 1979, 1980*a*; Bak & von Boehm 1980), it seems most probable that the ferromagnetic phase is bounded by the $\langle 3\rangle$ phase only up to a certain value of T and δ, say T_F and δ_F. For $T > T_F$ the the adjacent phase or phases seem to be 'sinusoidal' with wavelengths $\lambda(T, \delta) > \lambda_{\langle 3\rangle}$. However, it is by no means clear whether λ goes to infinity continuously as the ferromagnetic phase is approached for $T > T_F$. In any case, one may be tempted to identify T_F and δ_F with some characteristic behaviour such as the vanishing of $\Sigma_0(T)$ which might indicate some sort of continuous transition for $T > T_F$. We have therefore calculated

$\Sigma_0(T)$ numerically along $\delta_0(T)$ in first order and second order without expansion in powers of $w^{q_\perp}$: see figure 2. In second order the vanishing of Σ_0 occurs only at $\delta \approx -0.23$, which is close to the Lifshitz point in the model (see Redner & Stanley 1977; Selke 1978; Hornreich 1980). Thus the calculations give no indication of a continuous transition from a sinusoidal to the ferromagnetic phase. Indeed, while the wavelength of the modulated phase certainly seems to increase on lowering the temperature at constant δ (Selke & Fisher 1979, 1980*a*; Bak & von Boehm 1980), it may still jump discontinuously *at* the transition to the ferromagnetic phase (Bak & von Boehm 1980). One might, perhaps, speculate that the maximum in $\Sigma_0(T)$ at $\delta \approx -0.1$ locates δ_F; however, a low temperature calculation of Σ_0 to higher orders is clearly desirable to shed more light on these questions.

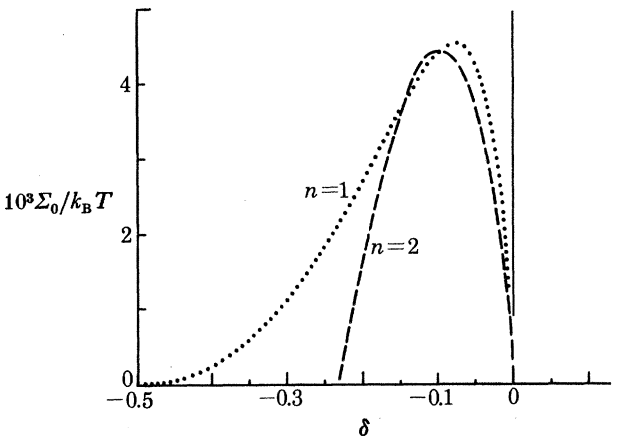

FIGURE 2. The interfacial tension $\Sigma_0(T)$ between the ferromagnetic and $\langle 3\rangle$ phases in second order (broken curve) and in first order (dotted curve) of the low temperature expansions ($J_0 = J_1$ on the simple cubic lattice).

6. INTERFACIAL ENERGY IN FERRO-PHASE

As a short further digression on the nature of the ferro-phase, we also calculate the interfacial tension, $\Sigma_{\langle\infty\rangle}(T)$, associated directly with the coexistence of two ferromagnetic domains separated by a plane perpendicular to the anisotropy axis. Thus consider a structure, where the first half of the layers point 'down' while the second half point 'up', $\langle -, +\rangle$. By arguments analogous to those yielding (5.4) one has

$$\Sigma_{\langle\infty\rangle}/k_B T = \tfrac{1}{2}(f_{\langle -,+\rangle} - f_{\langle\infty\rangle}). \tag{6.1}$$

A second-order calculation is not entirely trivial and uses the techniques explained further below: it yields

$$\begin{aligned}\Sigma_{\langle\infty\rangle}/k_B T = &-4K_1\delta - 2w^{q_\perp}(1 - 2x^{1-2\delta} + x^2) - q_\perp w^{2q_\perp - 2}(1 - 2x^{2-4\delta} + x^4)\\ &+ w^{2q_\perp}[q_\perp + 5x^{-4\delta} - 2x^{1-2\delta} + x^2 - (2q+9)x^{2-4\delta}\\ &+ 10x^{3-2\delta} + (q-3)x^4] + O(w^{3q_\perp - 4}).\end{aligned} \tag{6.2}$$

The vanishing of $\Sigma_{\langle\infty\rangle}(w, x; \delta)$ must signal the internal instability of the ferro-phase and hence must yield an upper bound for the domain of its existence in the (T, κ) plane. This yields a locus δ_Σ satisfying

$$K_1\delta_\Sigma = -\tfrac{1}{2}w^{q_\perp}(1 - x^2)[1 + O(w^{2q_\perp - 2})]. \tag{6.3}$$

Comparison with (5.3) at fixed T yields $\delta_0 < \delta_\Sigma$, which shows that the ferro-phase remains internally stable on the $\langle\infty\rangle\langle 3\rangle$ boundary, $\delta_0(T)$.

7. The $\langle 3\rangle$–$\langle 2\rangle$ region

The arguments of §4 lead to an expression, (4.6), for the free energy correct to order $w^{q_\perp}$ corresponding to an accounting of all single spin-flip excitations about all possible ground states. Thereby we established a region of stability, satisfying $\delta_0 \equiv \delta_{-\infty}(T) < \delta < \delta_1^{(1)}(T)$, at low but nonzero temperatures for a new equilibrium phase, $\langle 3\rangle$, a (3, 3) antiphase state, between the ferro- or $\langle\infty\rangle$ phase at sufficiently negative δ and the $\langle 2\rangle$ or (2, 2) antiphase at sufficiently positive δ. Examination of the $\langle\infty\rangle\langle 3\rangle$ boundary, $\delta = \delta_0(T)$, revealed that the transition was of first order with a positive surface tension $\Sigma_0(T)$ between the phases: no other phases can have a lower free energy in the vicinity of $\delta_0(T)$ at low T.

The situation on the border between the $\langle 3\rangle$ and $\langle 2\rangle$ phases is, however, quite different, Indeed, on extending the free energy calculations to higher order by overturning two and more spins, one discovers regions of stability in the vicinity $\delta = \delta_1^{(1)} + O(w^{2q_\perp})$, for further new phases of more complex structure. To understand this, first note from (4.6) that the condition (4.9), namely $a_2(\delta_1^{(1)}) = 0$, means that, for $\delta = \delta_1^{(1)}$ and to the leading order quoted, all phases based on structures with $l_k = 0$ for $k = 1$ and $k \geqslant 4$ will have the same free energy. This allows an infinite set of structures consisting only of 2-bands and 3-bands. *Henceforth*, therefore, *we need consider only such* 2:3 *phases*.

In making this assertion we are assuming here, as in §4, that the temperature is sufficiently low ($w \ll 1$) that higher-order powers of w (arising from multi-spin flip excitations) will not, for $d > 2$, alter the conclusions following from leading order. This corresponds roughly to asserting the convergence of the power series in w for the free energies of the stable phases for small enough w (and all $x \leqslant 1$ where we may note that $x = 1$ corresponds simply to *decoupled* layers): there seems no good reason to doubt such convergence for Ising systems of this sort.

On the other hand, taking account of the higher-order terms may maximize f for particular 2:3 phases in the vicinity $\delta = \delta_1^{(1)} + O(w^{2q_\perp})$, even at arbitrarily small temperatures. A schematic illustration of the mechanism responsible for this may be helpful at this point. Thus suppose that in next leading order one has for the pure $\langle 2\rangle$ state the expansion

$$f_{\langle 2\rangle} = A_2\,\delta + B_2 w^{q_\perp} + C_2 w^{2q_\perp} + \ldots, \tag{7.1}$$

in the vicinity of the locus $\delta = \delta_1^{(1)}(T)$ defined by $a_2(\delta_1^{(1)}) = 0$, while for some new, mixed, 2:3 state, say '1', the expansion is

$$f_1 = A_1\,\delta + B_1 w^{q_\perp} + C_1 w^{2q_\perp} + \ldots . \tag{7.2}$$

Equality of the two free energies to order $w^{q_\perp}$ on $\delta = \delta_1^{(1)}$ and the inequalities $B_1 > B_2$ and $A_1 < A_2$ ensure that the free energy $f_{\langle 2\rangle}$ will be larger than f_1 in the *same* order for $\delta > \delta_1^{(1)}(T)$. However, in next order it is clear that, if C_2 is smaller than C_1, then there will be a vicinity, $\delta = \delta_1^{(1)} + O(w^{2q_\perp}) > \delta_1^{(1)}$, in which f_1 exceeds $f_{\langle 2\rangle}$. In this case the stability of the $\langle 2\rangle$ phase cannot extend all the way down to the locus $\delta_1^{(1)}(T)$, and one must conclude that at least one new phase will be stable *between* the phases $\langle 2\rangle$ and $\langle 3\rangle$ (even though the phase $\langle 2\rangle$ remains stable for larger values, $\delta = \delta_1 + O(w^{q_\perp})$). This is the basic line of argument on which our analysis will rest. (In actual fact a term of order $w^{2q_\perp - 2}$ also appears, but that does not alter the

validity of the argument: see §9 for the exact expressions corresponding generally to (7.1) and (7.2)).

8. The 2:3 structural variables

The considerations presented so far establish that, at sufficiently low temperatures and for $\delta > 0$, to which we henceforth restrict attention, the only possible equilibrium phases are of 2:3 character, i.e. based on ground state structures consisting only of 2-bands and 3-bands. To describe such restricted structures we specialize the general definition of structural sequences and variables introduced in §2.

Specifically, let μ now be a binary sequence of twos and threes of length $m(\mu) \geqslant 1$, representing a corresponding sequence of 2-bands and 3-bands in a ground state structure. In accordance with (3.1), define the *structural variables* $l_\mu \equiv [\mu]$, so that $L_\mu = l_\mu L$ is the number of band sequences of type μ in a given structure or configuration in a lattice of L layers: for example, $L_{23} = l_{23}L$ is the number of *layers* in a 2-band followed immediately (going, say, to the 'right' or along the positive sense of the anisotropy axis) by a layer in a 3-band: note that $l_{32} = L_{32}/L$ is defined conversely and is *not* obviously equal to l_{23}, since there is no necessary right–left or positive–negative symmetry along the anisotropy axis. (However, in this special case, the equality $l_{32} = l_{23}$ can be established generally (see below); but it is easy to check that $l_{2233} \neq l_{3322}$ in the periodic structure $\langle 223323 \rangle$ for which l_{3322} vanishes!)

The following elementary result concerning the structural variables will be useful later:

Lemma 1: Basic structural lemma. *Suppose μ_- is a coherent subsequence of μ* (which may be improper, so that $\mu_- \equiv \mu$, but can have no 'gaps') *and that $l_\mu > 0$ in some lattice structure. Then in any such structure one also has $l_{\mu_-} > 0$.*

Proof. Since μ_- is a definite subsequence of μ, for each of the L_μ occurrences of a band sequence μ in the lattice, there will evidently also be at least one sequence μ_-. Thus, in fact, we have $l_{\mu_-} \geqslant l_\mu > 0$.

As mentioned before, it is clear that the structural variables l_μ cannot be chosen independently in any realizable lattice structure. Indeed, for length $m(\mu) = 1$, we must, by (3.2), have the relation

$$2l_2 + 3l_3 = 1. \tag{8.1}$$

We may thus choose l_2 as the independent (or 'standard') variable. In general, one needs only $2^{m(\mu)-2}$ out of the $2^{m(\mu)}$ distinct structural variables to describe structural sequences of length $m(\mu)$. To prove this, consider the *core*, $\tilde{\mu}$, of a structural sequence μ defined for $m(\mu) > 2$ by removing from μ its first and last symbol or corresponding first and last bands. There are four distinct structural variables of length $m(\mu)$ based on this core, namely $[2\tilde{\mu}2]$, $[2\tilde{\mu}3]$, $[3\tilde{\mu}2]$, and $[3\tilde{\mu}3]$. However, by considering the occurrence of the corresponding band sequences in an overall 2:3 structure, it is easy to see that these must satisfy the relations

$$\begin{aligned} [2\tilde{\mu}2] + [2\tilde{\mu}3] &= [2\tilde{\mu}], & [2\tilde{\mu}3] + [3\tilde{\mu}3] &= [\tilde{\mu}3], \\ [3\tilde{\mu}3] + [3\tilde{\mu}2] &= [3\tilde{\mu}], & [2\tilde{\mu}2] + [3\tilde{\mu}2] &= [\tilde{\mu}2], \end{aligned} \tag{8.2}$$

since every band sequence must be followed or preceded by either a 2-band or a 3-band. The new structural variables of length $m(\mu) - 1$ likewise must satisfy

$$[2\tilde{\mu}] + [3\tilde{\mu}] = [\tilde{\mu}], \qquad [\tilde{\mu}2] + [\tilde{\mu}3] = [\tilde{\mu}]. \tag{8.3}$$

It follows from these last relations that only three of the four relations (8.2) are independent. These suffice, however, to express all the structural variables based on the core $\tilde{\mu}$ in terms of any one of them (together with lower-order variables). Consequently, there are only $2^{m(\mu)-2}$ independent structural variables for length $m(\mu)$; by induction, a total number o 2^{m-1} independent structural variables suffice to describe all possible band-sequences μ of length m or less.

We will, shortly, introduce a criterion for the selection of a certain minimal set of *standard structural variables*, l_ν. In terms of these, we then have the general *structural relations*

$$l_\mu = \sum_\nu c_{\mu\nu} l_\nu, \tag{8.4}$$

where $c_{\mu\nu} = 0$ if $m(\nu) > m(\mu)$, and the sum runs only over the standard variables. It is convenient to present here the first few of these relations explicitly, the standard structural variables being those appearing on the right-hand sides:

$$l_3 = \tfrac{1}{3} - \tfrac{2}{3} l_2, \tag{8.5}$$

$$l_{22} = l_2 - l_{23}, \qquad l_{32} = l_{23}, \qquad l_{33} = \tfrac{1}{3} - \tfrac{2}{3} l_2 - l_{23}; \tag{8.6}$$

and, for $m = 3$, two sets based on the cores 2 and 3, respectively:

$$l_{222} = l_2 - l_{23} - l_{223}, \qquad l_{322} = l_{223}, \qquad l_{323} = l_{23} - l_{223}, \tag{8.7}$$

$$l_{232} = l_{23} - l_{233}, \qquad l_{332} = l_{233}, \qquad l_{333} = \tfrac{1}{3} - \tfrac{2}{3} l_2 - l_{23} - l_{233}; \tag{8.8}$$

while the first set for $m = 4$, based on the core 22, is

$$l_{2^4} = l_2 - l_{23} - l_{223} - l_{2223}, \tag{8.9}$$

$$l_{32^3} = l_{2223} \equiv l_{2^3 3}, \tag{8.10}$$

$$l_{32^2 3} = l_{223} - l_{2223}, \tag{8.11}$$

in which we have introduced the convenient shorthand notation

$$2^j \equiv 22\ldots2 \ (j \text{ symbols}), \quad 3^{j'} \equiv 33\ldots3 \ (j' \text{ symbols}), \tag{8.12}$$

in writing the longer sequences μ. The other standard variables for $m = 4$ are $l_{2233} \equiv l_{2^2 3^2}$, $l_{3322} \equiv l_{3^2 2^2}$ and $l_{2333} \equiv l_{2 3^3}$: the corresponding relations are easily constructed.

It is useful to introduce the *span*, $n_0(\mu)$, of a structural sequence μ to allow for the fact that second-neighbour axial neighbouring spins interact directly so that, when two such spins are overturned, their contribution to the partition function expansion is different from that if they are further separated. Thus we define $n_0(\mu)$ as the *minimum number of overturned spins in a set linked by first- or second-neighbour (axial) bonds such that there is an overturned spin in both the first and last band specified by* μ.

Thence we find $n_0(\mu) = m(\mu)$ for $m(\mu) \leqslant 3$. However, at length $m = 4$ one has, for example, $n_0(2^4) = 4$ but $n_0(2332) = 5$, as is easily verified by drawing appropriate diagrams. In fact, $n_0(\mu)$ depends only on the core $\tilde{\mu}$. If the core contains just a single 3-band, the structural sequence can be spanned by $m(\mu)$ spins provided the 3-band is occupied by a centre or ρ-type spin [see (2.5)]. However, the presence of two 3-bands in the core requires a ρ spin and two edge or σ-type spins so that $m(\mu) + 1$ spins are needed to span μ, and so on. Generally each 2-band in the core requires only one edge or τ-type spin. In total, therefore, we find

$$n_0(\mu) = 2 + \tilde{m}_2 + \{\tfrac{3}{2}\tilde{m}_3\} = m(\mu) + \{\tfrac{1}{2}\tilde{m}_3(\mu)\}, \tag{8.13}$$

where $\tilde{m}_k(\mu)$ is the number of k-bands in the core of μ while $\{z\}$ is the greatest integer contained in z. Note that $m(\mu) \leqslant n_0(\mu) \leqslant \frac{3}{2}m(\mu) - 1$ for $m(\mu) \geqslant 2$.

To choose the 2^{m-2} *standard structural sequences*, ν, needed to specify all sequences of length m or less, we introduce conventions whose usefulness will appear only when we proceed to establish the particular sequence of 2:3 phases that actually occurs in equilibrium at low temperatures. The main point is to select sequences, ν, that cannot be generated by periodic repetition of some lower-order ν' with $m(\nu') < m(\nu)$ so that l_ν will vanish identically in a structure $\langle \nu' \rangle$. These are 'nonperiodic sequences'. The first example of a bad choice would be $\nu = \mu = 2323$ at $m = 4$, since this satisfies $\mu = \nu'\nu'$ with $\nu' = 23$. Similarly, we wish to avoid, as far as possible, 'subperiodic sequences', μ, which are defined so that l_μ does not vanish in some lower-order periodic structure $\langle \mu' \rangle$ with $m(\mu') < m(\mu)$. More specifically, μ' must not correspond to an *extremal vertex* of the *structural polytopes* that will be introduced in §§10 and 11. An important example of a subperiodic structure is provided by $\mu = 2^{j-1}32^j3$, where one has $l_\mu > 0$ for the structure $\langle \mu' \rangle$ with $\mu' = 2^j3$.

To these ends we first adopt *convention* A in which the standard sequences ν of length m are formed from all possible 2^{m-2} sequences of length $m-2$, i.e. from the cores, $\tilde{\nu}$, according to the rule

$$\text{(A)} \qquad \nu = 2\tilde{\nu}3. \tag{8.14}$$

In addition, for the cases $m = 1$ and 2, we choose $\nu = 2$ and $\nu = 23$, respectively (see (8.5) and (8.6)). It is then convenient to list the ν in lexicographical order by their cores $\tilde{\nu}$.

However, to avoid generating periodic and subperiodic structures (which arise first on convention A already for $\tilde{\nu} = 32$, as shown above), we add *convention* B, which replaces such structures by the alternative

$$\text{(B)} \qquad \nu = 3\tilde{\nu}2. \tag{8.15}$$

It can be shown that this convention avoids subperiodic standard structures of length $m \leqslant 7$: however, for $m = 8$ the core $\tilde{\mu} = 233223$ generates a sub-periodic structure ν on either convention. Nevertheless, for the cases that play a crucial role in the general arguments in §§10 and 11, these two conventions suffice. To order $m = 6$ they yield the standard sequences that we record here for reference:

$$m = 1\colon\ \nu = 2; \quad m = 2\colon\ \nu = 23; \quad m = 3\colon\ \nu = 223, 233; \tag{8.16}$$

$$m = 4\colon\ \nu = 2223, 2233, 2333 \mid 3322; \tag{8.17}$$

$$m = 5\colon\ \nu = 2^43, 2^33^2, 2^2323, 2^23^3, 2323^2, 23^4 \mid 3^22^3, 3^32^2; \tag{8.18}$$

$$m = 6\colon\ \nu = 2^53, 2^43^2, 2^3323, 2^33^3, 2^2323^2, 2^23^223, 2^23^4, 232^23^2,$$
$$2323^3, 23^5 \mid 3232^3, 3^22^4, 3^22322^2, 3^32^3, 3^3232, 3^42^2. \tag{8.19}$$

Note that the standard sequences after the vertical bars follow from convention B.

9. Low temperature expansions to third order

The line of attack is now clear: the free energy for all possible 2:3 structures must be calculated as a power series in w with coefficients depending on x, δ, and the standard variables l_ν, which must then be varied to yield the lowest free energy. Now the explicit calculations to

order $w^{q_\perp}$, based on the decomposition (4.3) of the partition function $Z_N\{l_\mu\}$ in terms of contributions from $n = 1, 2, \ldots$ overturned spins, lead to the expression (4.6) for the reduced free energy, $f\{l_\mu\}$, which is *linear in the structural variables*, l_μ. The reasons for this linearity are as follows. (*a*) The contributions to the ground state energy of a given type of spin and the energy, ϵ_ω, of an excited state configuration ω of overturned spins depend only on the local environment of the spins in ω out to first neighbours within a layer and out to second neighbours along the anisotropy axis. (*b*) The nature of all local environments can be described adequately by specifying the appropriate structural variables. Indeed, it is clear from the previous section that for a configuration of $n(\omega)$ overturned spins one needs only standard structural variables, l_ν, of *span* satisfying $n_0(l_\nu) \leqslant n$. (*c*) The configurational counts, N_ω, specifying the number of occurrences of a configuration ω on a lattice of structure given by $\{l_\mu\}$ can be expressed explicitly in terms of the appropriate variables l_ν. (*d*) The single-spin counts, N_λ, needed to describe the ground state and $n = 1$ excited states included in (4.6), are just linear functions of the l_ν.

Now the features (*a*), (*b*) and (*c*) above hold quite generally for all n, but the last condition (*d*) will certainly be violated for states of $n \geqslant 2$ overturned spins. Nevertheless, *the free energy in all orders remains a linear function of the standard structural variables*, l_ν.

To see this† consider, for example, the number $N_{\rho;\rho}$ of *separated configurations* of two overturned spins, of type ρ, i.e. centre spins in a 3-band (see (2.5)); here 'separated' means that the two overturned spins are not 'linked' or 'connected' by any of the interaction bonds of strength J_0, J_1, or J_2 in $\mathscr{H}$ (see also Domb 1960). If N_ρ [$= Nl_3$, see (3.5)] is the number of ρ spins in a structure, then a little consideration yields

$$N_{\rho;\rho} = \tfrac{1}{2}N_\rho(N_\rho - 1) - N_{\rho\rho}, \tag{9.1}$$

where $N_{\rho\rho}$ denotes a connected configuration, $(\rho\rho)$, of two neighbouring spins in the same layer; for this, in turn, one easily concludes

$$N_{\rho\rho} = \tfrac{1}{2}q_\perp N_\rho = \tfrac{1}{2}q_\perp Nl_3. \tag{9.2}$$

On combining these expressions and going over to the standard structural variable l_2 (see (8.5)), we obtain

$$N_{\rho;\rho} = \tfrac{1}{18}N^2(1 - 4l_2 + 4l_2^2) - \tfrac{1}{6}N(q_\perp + 1)(1 - 2l_2), \tag{9.3}$$

which is evidently nonlinear in l_2. However, the coefficient of l_2^2 is proportional to N^2, and, more generally, it should be clear from this example that the coefficients of *any* nonlinear terms in the structural variable expressions for any configurational count, N_ω, will be proportional to N^2 or a higher power of N. But, while the configurational counts N_ω enter linearly into the expansions for the partial partition functions, $\Delta Z_N^{(n)}$, one actually wants to compute the reduced free energy per spin defined by

$$f\{l_\mu\} = N^{-1} \ln \left[1 + \sum_{n=1} \Delta Z_N^{(n)}\right]. \tag{9.4}$$

As is well known (see, for example, Domb 1960) the contributions to the free energy expansion from terms in the N_ω proportional to $N^2, N^3, \ldots$ cancel exactly on taking the logarithm (a 'linked cluster' theorem). Thus all that is actually required from an expression for a configurational count like (9.3) is the coefficient of the term linear in N. Again, it is clear from the

† The reader willing to accept this crucial result may wish to proceed directly to the next section where the general development continues.

example that such a coefficient can at most vary linearly with the structural variables. In the present case the contribution of the configuration $\omega = (\rho; \rho)$ to the reduced free energy is thence found to be

$$(\rho; \rho) \Rightarrow [-\tfrac{1}{6}(q-1) + \tfrac{1}{3}(q-1)\, l_2]\, w^{2q_\perp} x^{6+4\delta}, \tag{9.5}$$

where the Boltzmann factor, $\exp(-\epsilon_{\rho;\rho}/k_B T)$, follows from the observation

$$\epsilon_{\lambda;\lambda'} = \epsilon_\lambda + \epsilon_{\lambda'}, \tag{9.6}$$

valid for any separated configuration of two single spins, and the results (4.1) and (3.8); we have also used $q_\perp = q-2$.

TABLE 1. LIST OF CONFIGURATIONS, COUNTS AND BOLTZMANN WEIGHTS FOR THE SECOND-ORDER (TWO SPIN-FLIP) CONTRIBUTIONS TO THE FREE ENERGY

configuration, ω	count, N_ω	weight
separated		
$\rho;\rho$	$\frac{1}{2}N_\rho(N_\rho-1) - N_{\rho\rho}$	$w^{2q_\perp}x^{6+4\delta}$
$\sigma;\sigma$	$\frac{1}{2}N_\sigma(N_\sigma-1) - N_{\sigma\sigma} - N_{\sigma\cdot\sigma} - N_{\sigma/\sigma}$	$w^{2q_\perp}x^{0}$
$\tau;\tau$	$\frac{1}{2}N_\tau(N_\tau-1) - N_{\tau\tau} - N_{\tau\cdot\tau} - N_{\tau/\tau} - N_{\tau,\tau}$	$w^{2q_\perp}x^{2+4\delta}$
$\rho;\sigma$	$N_\rho N_\sigma - N_{\rho,\sigma} - N_{\rho\cdot\sigma}$	$w^{2q_\perp}x^{3+2\delta}$
$\rho;\tau$	$N_\rho N_\tau - N_{\rho\cdot\tau}$	$w^{2q_\perp}x^{4+4\delta}$
$\sigma;\tau$	$N_\sigma N_\tau - N_{\sigma/\tau} - N_{\sigma\cdot\tau}$	$w^{2q_\perp}x^{4+2\delta}$
in-layer		
$\rho\rho$	$\frac{1}{6}q_\perp(1-2l_2)\ N$	$w^{2q_\perp-2}x^{6+4\delta}$
$\sigma\sigma$	$\frac{1}{3}q_\perp(1-2l_2)\ N$	$w^{2q_\perp-2}x^{0}$
$\tau\tau$	$q_\perp l_2 N$	$w^{2q_\perp-2}x^{2+4\delta}$
axial close (*in-band*)		
ρ,σ	$\frac{2}{3}(1-2l_2)\ N$	$w^{2q_\perp}x^{1+2\delta}$
τ,τ	$l_2 N$	$w^{2q_\perp}x^{4\delta}$
(*cross-band*)		
σ/σ	$(\frac{1}{3}-\frac{2}{3}l_2-l_{23})\ N$	$w^{2q_\perp}x^{2}$
σ/τ	$2l_{23} N$	$w^{2q_\perp}x^{3+2\delta}$
τ/τ	$(l_2-l_{23})\ N$	$w^{2q_\perp}x^{4+4\delta}$
axial spaced		
$\sigma\cdot\sigma$	$\frac{1}{3}(1-2l_2)\ N$	$w^{2q_\perp}x^{1+2\delta}$
$\rho\cdot\sigma$	$2(\frac{1}{3}-\frac{2}{3}l_2-l_{23})\ N$	$w^{2q_\perp}x^{2}$
$\rho\cdot\tau$	$2l_{23} N$	$w^{2q_\perp}x^{3+2\delta}$
$\sigma\cdot\tau$	$2l_{23} N$	$w^{2q_\perp}x^{0}$
$\tau\cdot\tau$	$2(l_2-l_{23})\ N$	$w^{2q_\perp}x^{1+2\delta}$

The conclusion (9.5) represents the first step in the general calculation of the second-order (two spin-flip) contribution to the free energy, $\Delta f^{(2)}$. To complete the calculation, note first that in the 2:3 phases only spins of types ρ (centre), σ (edge), and τ (2-band) can enter [see (2.5)]. Then one must enumerate all possible types of spin configuration. If we allow for general orientation in the counts, we find a total of *six* distinct separated configurations: *three* in-layer connected configurations like $(\rho\rho)$; *five* configurations linked as first neighbours axially, either in the *same* band, which we denote, for example, by (ρ, σ), or *across* a band, which are written, for example, (σ/τ); and, finally, *five* second-neighbour axial configurations which are indicated $(\rho\cdot\sigma)$. The total of 19 configurations and their corresponding counts and weights are listed in table 1.

TABLE 2. COEFFICIENTS $a_\mu^{(2;\alpha,\beta)}$ FOR THE FREE ENERGY EXPANSION IN SECOND ORDER

$\mu = 0$	$\mu = 2$	$\mu = 23$	α†	β
$\frac{1}{3}q_\perp$	$-\frac{2}{3}q_\perp$	—	$2q_\perp-2$	0
0	$q_\perp$	—		$2+4\delta$
$\frac{1}{6}q_\perp$	$-\frac{1}{3}q_\perp$	—		$6+4\delta$
$-\frac{1}{3}(q+1)$	$\frac{2}{3}(q+1)$	3	$2q_\perp$	0
0	1	0		4δ
1	0	-6		$1+2\delta$
1	-2	-3		2
0	$-q-3$	3		$2+4\delta$
$-\frac{4}{3}$	$\frac{8}{3}$	6		$3+2\delta$
0	1	-3		$4+4\delta$
$-\frac{1}{6}(q-1)$	$\frac{1}{3}(q-1)$	0		$6+4\delta$

† Note that blank entries under α denote the same value as the top of the column.

TABLE 3. COEFFICIENTS FOR THE FREE ENERGY EXPANSION IN THIRD ORDER: $a_\mu^{(3;\alpha,\beta)}$

Note: $q_1 = q-1 = q_\perp+1$ and $c_2 = \frac{1}{2}q_\perp(q-3)-p_3$, where p_3 is the number of triangles per site.

$\mu = 0$	$\mu = 2$	$\mu = 23$	$\mu = 223$	$\mu = 233$	α	β
$\frac{2}{3}p_3$	$-\frac{4}{3}p_3$				$3q_\perp-6$	0
0	$2p_3$					$3+6\delta$
$\frac{1}{3}p_3$	$-\frac{2}{3}p_3$					$9+6\delta$
$\frac{2}{3}c_2$	$-\frac{4}{3}c_2$				$3q_\perp-4$	0
0	$2c_2$					$3+6\delta$
$\frac{1}{3}c_2$	$-\frac{2}{3}c_2$					$9+6\delta$
$2p_3-\frac{2}{3}qq_\perp$	$\frac{4}{3}qq_\perp-4p_3$	$4q_\perp$			$3q_\perp-2$	0
$\frac{4}{3}q_\perp$	$-\frac{8}{3}q_\perp$	$-2q_\perp$				$1+2\delta$
0	$2q_\perp$	0				$1+6\delta$
$\frac{4}{3}q_\perp$	$-\frac{8}{3}q_\perp$	$-4q_\perp$				2
0	$4q_\perp$	$-8q_\perp$				$2+4\delta$
$-\frac{4}{3}q_\perp$	$\frac{8}{3}q_\perp$	$4q_\perp$				$3+2\delta$
0	$6p_3-2q_\perp^2-8q_\perp$	$6q_\perp$				$3+6\delta$
$\frac{2}{3}q_\perp$	$-\frac{4}{3}q_\perp$	$4q_\perp$				$4+4\delta$
$\frac{2}{3}q_\perp$	$-\frac{4}{3}q_\perp$	$-2q_\perp$				$5+2\delta$
0	$q_\perp$	$-4q_\perp$				$5+6\delta$
$-\frac{4}{3}q_\perp$	$\frac{8}{3}q_\perp$	$4q_\perp$				$6+4\delta$
0	0	$-2q_\perp$				$7+6\delta$
$p_3-\frac{1}{3}q_\perp^2$	$\frac{2}{3}q_\perp^2-p_3$	0				$9+6\delta$
$\frac{1}{3}q(q+1)-\frac{2}{3}p_3+\frac{8}{9}$	$\frac{4}{3}p_3-\frac{2}{3}q(q+1)-\frac{16}{9}$	$-4(q+1)$	4		$3q_\perp$	0
$\frac{1}{3}$	$\frac{4}{3}$	-4	0			4δ
$\frac{1}{3}$	$-\frac{2}{3}$	-1	0	-1		$1-2\delta$
$-\frac{4}{3}(q+1)$	$\frac{2}{3}(4q+7)$	$2(q+7)$	-12			$1+2\delta$
0	$-2q-2$	4			$3q_\perp$	$1+6\delta$
$-\frac{4}{3}(q+1)$	$\frac{8}{3}(q+1)$	$4(q+2)$	-4	4		2
0	$-4(q+1)$	$8q-4$	12	0		$2+4\delta$
$\frac{1}{3}(4q+11)$	$-\frac{2}{3}(4q+13)$	$-4q-22$	12	-6		$3+2\delta$
0	$q(q+5)-2p_3+\frac{14}{3}$	$-6(q+1)$	-4	0		$3+6\delta$
$-\frac{2}{3}q-1$	$\frac{4}{3}(q+3)$	$-4(q-3)$	-12	4		$4+4\delta$
$-\frac{2}{3}(q+1)$	$\frac{4}{3}(q+1)$	$2(q+1)$	0	0		$5+2\delta$
0	$-2(q+1)$	$4q+3$	4	-1		$5+6\delta$
$\frac{2}{3}(2q-1)$	$-\frac{4}{3}(2q-1)$	$-4q$				$6+4\delta$
0	0	$2(q-1)$				$7+6\delta$
$\frac{1}{6}q_1q_\perp-\frac{1}{3}p_3+\frac{1}{9}$	$\frac{2}{3}p_3-\frac{1}{3}q_1q_\perp-\frac{2}{9}$	0				$9+6\delta$

From this table and the results of §4 one can construct the expansions

$$\Delta f_{2:3}^{(0)} = \tfrac{1}{2}q_\perp K_0 + \tfrac{1}{2}K_1 + \tfrac{1}{3}K_1\,\delta + \tfrac{4}{3}K_1\,\delta l_2, \tag{9.7}$$

$$\Delta f_{2:3}^{(1)} = \tfrac{1}{3}(2 + x^{3+2\delta})\,w^{q_\perp} - \tfrac{2}{3}(2 - 3x^{1+2\delta} + x^{3+2\delta})\,w^{q_\perp} l_2, \tag{9.8}$$

$$\Delta f_{2:3}^{(2)} = \sum_\alpha [a_0^{(2;\alpha)} + a_2^{(2;\alpha)} l_2 + a_{23}^{(2;\alpha)} l_{23}]\,w^\alpha, \tag{9.9}$$

which involve only the first two standard structural variables. The coefficients in the second order and analogous higher expressions may be written

$$a_\mu^{(n;\alpha)} = \sum_\beta a_\mu^{(n;\alpha,\beta)} x^{\beta(\delta)}, \tag{9.10}$$

where the exponents α and $\beta(\delta)$ run over only certain allowed values: in particular, $\alpha_{\min} = p_0(n)$ (see §4) and $\alpha_{\max} = nq_\perp$, while the β are linear in δ, and the α depend only on $q_\perp$. The basic coefficients $a_\mu^{(n;\alpha,\beta)}$ derived from table 1 are presented in table 2.

The corresponding third-order results are listed in table 3 and involve the four standard structural variables l_2, l_{23}, l_{223}, and l_{233}. The derivation of these coefficients requires the analysis of 96 distinct spin configurations which may be grouped into six classes:

(i) Three completely separated spins, e.g. $(\rho;\,\sigma;\,\sigma)$.

(ii) Two spins neighbouring in a layer and one separated, e.g. $(\tau\tau;\,\rho)$.

(iii) Two spins axially linked and one separated, e.g. $(\rho,\,\sigma;\,\tau)$, $(\sigma/\sigma;\,\rho)$, and $(\rho\cdot\tau;\,\tau)$.

(iv) Three spins linked as nearest neighbours in the same layer, e.g. $(\sigma\sigma\sigma)$.

(v) A pair of neighbouring spins in a layer linked axially to a third spin, e.g. $(\rho,\,\sigma\sigma)$ or $(\sigma/\tau\tau)$.

(vi) Three axially linked spins, e.g. $(\rho,\,\sigma/\tau)$, $(\rho,\,\sigma\cdot\tau)$, $(\sigma\cdot\sigma/\tau)$, and $(\rho\cdot\tau\cdot\sigma)$.

In table 3 the number of triangles per lattice site is denoted p_3 (so that, for example, $p_3 = 0$ on the simple cubic lattice), while the number of 2-chains per site is denoted c_2 and one has $c_2 = \tfrac{1}{2}q_\perp(q_\perp - 1) - p_3$ (see also Domb 1960).

The data presented in tables 1–3 represent the fruits of considerable labour and would not be easy to extend. They may, however, be checked in various limits such as $x = 1$.

As a result of the foregoing, we may write quite generally

$$f_{2:3}\{l_\mu\} = a_0(w, x;\,\delta) + \sum_\nu a_\nu(w, x;\,\delta)\,l_\nu, \tag{9.11}$$

where the sum runs over the standard structural variables, and the coefficients (for $\nu \neq 0$) can be expanded as

$$a_\nu(w, x;\,\delta) = \sum_\alpha a_\nu^{(\alpha)}(x;\,\delta)\,w^\alpha = \sum_{n;\,\alpha,\,\beta} a_\nu^{(n;\alpha,\beta)} x^{\beta(\delta)} w^\alpha. \tag{9.12}$$

Furthermore, to determine the excitation energies, ϵ_ω, and hence the exponents α and β, it is clear that fully axial configurations, in which all n overturned spins are linked along an axis, place the greatest demand on the length of the structural sequences ν that are required. Such configurations have $q_\perp$ 'wrong' bonds in each of their n layers, so that $\alpha = nq_\perp$. On the other hand, it is not hard to check that ϵ_ω can be determined unambiguously, provided, as already mentioned, all structures of span $n_0(\nu) \leqslant n$ are known (see (8.13)). Consequently, we can write

$$a_\nu(w, x;\,\delta) = w^{n_0(\nu)q_\perp} b_\nu(w, x;\,\delta), \tag{9.13}$$

where b_ν contains no power of w of lower order than $w^{q_\perp - 2}$.

The expression (9.11) together with the constraints $l_\mu \geqslant 0$ (all μ) and the structural relations (8.4)–(8.11), confirm our assertion that the stable 2:3 phases can be found by solving a linear programming problem (see, for example, Wilf 1962, Gass 1964). In principle, our problem involves infinitely many standard variables, l_ν, but in view of the restriction (9.13) we may examine the stability of the phases and their borders in successive stages $n_0 = 1, 2, 3, \ldots$. Using the expansions now in hand let us, therefore, determine in second and third order the nature of the $\langle 2\rangle$–$\langle 3\rangle$ region. This will also serve to illustrate the general arguments developed in subsequent sections.

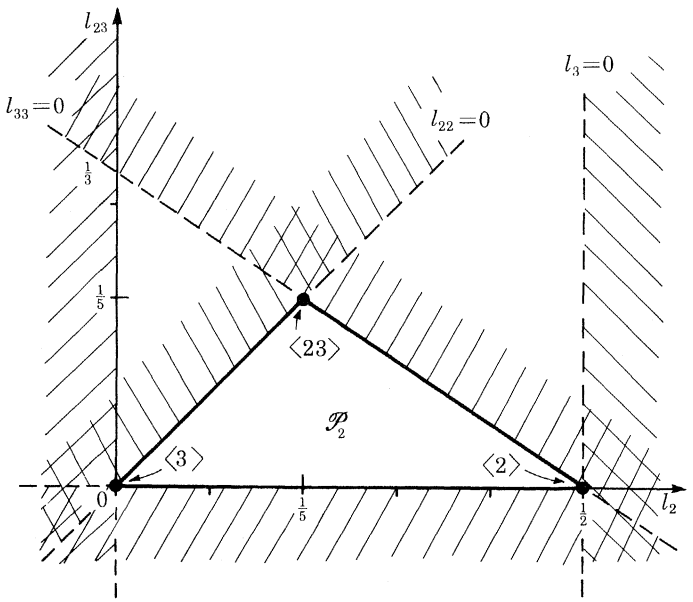

FIGURE 3. The structural polytope $\mathscr{P}_2$ in the plane (l_2, l_{23}) as determined by the set of structural inequalities. (The shaded areas correspond to $l_\mu < 0$ for some μ.) The vertices are labelled by the periodic phases they uniquely represent.

Consider the second-order stage $n_0 = 2$, where we require just the two variables l_2 and l_{23}, which define a *second-order structural space*, $\mathscr{L}_2$, illustrated explicitly in figure 3. Now the relevant inequalities in first order are, by (8.5),

$$l_2 \geqslant 0, \quad \text{and} \quad l_3 \equiv \tfrac{1}{3} - \tfrac{2}{3} l_2 \geqslant 0 \quad \text{or} \quad l_2 \leqslant \tfrac{1}{2}, \tag{9.14}$$

and, in second order, by (8.6),

$$l_{23} \geqslant 0, \quad l_{22} \equiv l_2 - l_{23} \geqslant 0, \quad l_{33} \equiv \tfrac{1}{3} - \tfrac{2}{3} l_2 - l_{23} \geqslant 0. \tag{9.15}$$

These inequalities are shown graphically in figure 3 and evidently define a convex polytope $\mathscr{P}_2$, which in this case is simply a triangle, with *vertices* $(l_2, l_{23}) = (0, 0)$, $(\frac{1}{5}, \frac{1}{5})$, and $(\frac{1}{2}, 0)$. A little thought shows that these vertices correspond uniquely to the *periodic structures* $\langle 3\rangle$, $\langle 23\rangle$, and $\langle 2\rangle$, respectively. This will prove to be a general feature.

Now it is a conclusion of linear programming theory (Wilf 1962, Gass 1964) that an objective function, in this case $f\{l_\nu\}$ to second order, will, in general (that is, 'generically'), be optimized or attain its maximum *on* a *unique* vertex of the convex polytope $\mathscr{P}$ defined by the inequalities. In the present case we thus conclude that, in addition to the two already-known equilibrium phases $\langle 3\rangle$ and $\langle 2\rangle$, a new commensurate phase, $\langle 23\rangle$, *might* have a region of

stability. To determine if $\langle 23\rangle$ can in fact be stable, i.e. to maximize $f\{l_\nu\}$, we must evaluate the expansion for f on the vertices. It is most straightforward, as before, to take x and w fixed (the latter, as always, being sufficiently small), and vary δ. We may anticipate that as δ varies the optimal or maximal vertex will change discontinuously, corresponding to a phase transition (at the stage considered). We may now appeal directly to the argument explained schematically in §7. We are concerned only with the vicinity of the locus $\delta_1^{(1)}(T)$ defined by

$$0 = a_2(\delta_1^{(1)}) = \tfrac{4}{3}K_1\,\delta_1^{(1)} - \tfrac{2}{3}w^{q_\perp}(2-3x+x^3) + O(w^{2q_\perp-2}), \tag{9.16}$$

where we have used the result $\delta_1^{(1)} = O(w^{q_\perp})$ (see (4.11)). Recall, that to *first order* in $w^{q_\perp}$ the phases $\langle 2\rangle$ and $\langle 3\rangle$ have equal free energies on the locus $\delta_1^{(1)}(T)$. Then we need (from the tables) only the result

$$a_{23}(\delta) = 3(1-x^2)\,(1-x^{1+2\delta})^2 w^{2q_\perp} + O(w^{3q_\perp-2}), \tag{9.17}$$

which is certainly *positive* (for small enough w and $x < 1$) when $\delta \approx \delta_1^{(1)}$. It is thus clear that by allowing for $l_{23} > 0$ we can increase f when $\delta = \delta_1^{(1)}(T)$ so that the vertex $\langle 23\rangle$ becomes maximal. By continuity this will also be true for δ in the vicinity of δ_1, specifically $\delta = \delta_1^{(1)}(T) + O(w^{2q_\perp})$. *Thus we have established the existence of* $\langle 23\rangle$ *as an equilibrium phase between* $\langle 3\rangle$ *and* $\langle 2\rangle$.

In the next stage we must clearly examine the two borders, $\delta_1^{(2)}$ and $\delta_2^{(2)}$, defined by the equalities

$$f_{\langle 3\rangle} = f_{\langle 23\rangle} \quad \text{and} \quad f_{\langle 23\rangle} = f_{\langle 2\rangle}, \tag{9.18}$$

to second order, respectively. By substituting the vertex values for l_2 and l_{23} into (9.11) to order $n_0 = 2$ these yield the equations

$$a_2(\delta_1^{(2)}) + a_{23}(\delta_1^{(2)}) = 0 \quad \text{and} \quad \tfrac{1}{2}a_2(\delta_2^{(2)}) + a_{23}(\delta_2^{(2)}) = 0. \tag{9.19}$$

Next one must examine the *third-order structural space*, $\mathscr{L}_3$, spanned by the four variables (l_2, l_{23}, l_{223}, l_{233}): this is exhibited in figure 4. In addition to the five inequalities (9.14) and (9.15), six further relevant inequalities follow from (8.7) and (8.8). The task of finding the corresponding polytope $\mathscr{P}_3$ as defined by these eleven inequalities is not entirely trivial. It may be accomplished algebraically by an exhaustive analysis leading to the result illustrated in figure 4. Alternatively, one may proceed numerically by using the simplex method (see, for example, Wilf 1962, Gass 1964) with a variety of trial objective functions. In practice we have used as objective functions linear combinations of subsets of the l_ν with coefficients ± 1. In principle such an explorative approach may miss certain vertices of the polytope $\mathscr{P}_n$ in stage n. However, for $n = 3$ it agrees precisely with the algebraic approach and yields the vertices shown in figure 4 which again turn out to describe only periodic structures, namely $\langle 3\rangle$, $\langle 2\rangle$, $\langle 23\rangle$, as before, and also $\langle 223\rangle$, $\langle 233\rangle$, and $\langle 2233\rangle$. In the next two stages each vertex found numerically arises from several trial functions, and one may be confident that all vertices have been found: see table 4: however, a *complete* analysis of the vertices proves not to be essential to the general arguments presented later.

At the third stage, then, three possible new phases, namely $\langle 223\rangle$, $\langle 233\rangle$, and $\langle 2233\rangle$, must be considered. Now after the previous line of argument, using (9.19), and noting that the coefficient

$$a_{223} = 4(1-x^2)\,(1-x^{1+2\delta})^3 w^{3q_\perp}[1+O(w^{q_\perp-2})] \tag{9.20}$$

is positive, we can conclude that $\langle 223\rangle$ *appears as a new stable equilibrium phase* in the vicinity $\delta = \delta_2^{(2)}(T) + O(w^{3q_\perp})$. Conversely the coefficient

$$a_{233} \approx -x^{1-2\delta}(1-x^{1+2\delta})^4 w^{3q_\perp} \tag{9.21}$$

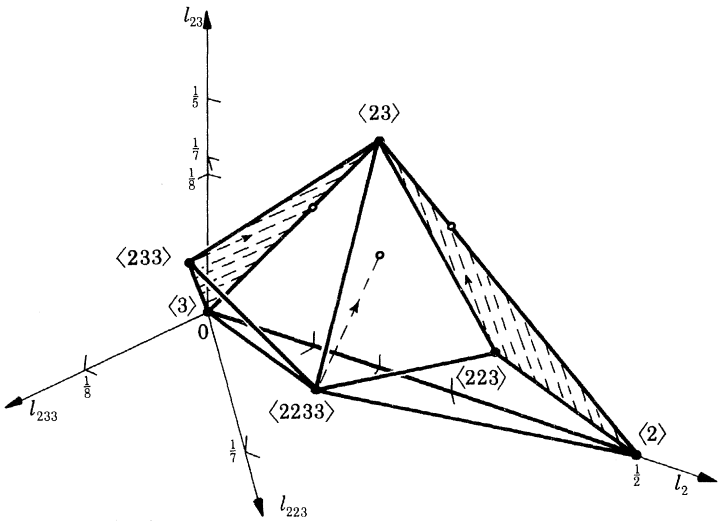

FIGURE 4. A view of the structural polytope, $\mathscr{P}_3$, projected on to a plane from the third-stage structural space, $\mathscr{L}_3$, with coordinates $(l_2, l_{23}, l_{223}, l_{233})$, as entailed in analysing configurations of three overturned spins. The open circles represent orthogonal projections of vertices on to the plane (l_2, l_{23}) which contains $\mathscr{P}_2$ (see figure 3). Note that the shaded triangles' faces project on to edges of $\mathscr{P}_2$.

TABLE 4. LIST OF VERTICES IN THE ⟨3⟩–⟨2⟩ REGION

standard structural coefficient values, l_ν†

order n_0	structure	2	23	223	233	2^33	23^3	2^23^2	3^22^2	2^43	2^33^2	2^2323	2^23^3	2323^2	23^4	3^22^3	3^32^2
1	⟨2⟩	$\frac{1}{2}$															
	⟨3⟩	0															
2	⟨23⟩	$\frac{1}{5}$	$\frac{1}{5}$														
3	⟨233⟩	$\frac{1}{8}$	$\frac{1}{8}$	0	$\frac{1}{8}$												
	⟨223⟩	$\frac{2}{7}$	$\frac{1}{7}$	$\frac{1}{7}$	0												
	⟨2233⟩	$\frac{1}{5}$	$\frac{1}{10}$	$\frac{1}{10}$	$\frac{1}{10}$												
4	$\langle 23^3\rangle$	$\frac{1}{11}$	$\frac{1}{11}$	0	$\frac{1}{11}$	0	$\frac{1}{11}$	0	0								
	$\langle 2^33\rangle$	$\frac{1}{3}$	$\frac{1}{9}$	$\frac{1}{9}$	0	$\frac{1}{9}$	0	0	0								
	$\langle 2^23^3\rangle$	$\frac{2}{13}$	$\frac{1}{13}$	$\frac{1}{13}$	$\frac{1}{13}$	0	$\frac{1}{13}$	$\frac{1}{13}$	$\frac{1}{13}$								
	$\langle 2^33^2\rangle$	$\frac{1}{4}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	0	$\frac{1}{12}$	$\frac{1}{12}$								
	$\langle 2^33^3\rangle$	$\frac{1}{5}$	$\frac{1}{15}$	$\frac{1}{15}$	$\frac{1}{15}$	$\frac{1}{15}$	$\frac{1}{15}$	$\frac{1}{15}$	$\frac{1}{15}$								
5	$\langle 2^43\rangle$	$\frac{4}{11}$	$\frac{1}{11}$	$\frac{1}{11}$	0	$\frac{1}{11}$	0	0	0	$\frac{1}{11}$	0	0	0	0	0	0	0
	$\langle 23^4\rangle$	$\frac{1}{14}$	$\frac{1}{14}$	0	$\frac{1}{14}$	0	$\frac{1}{14}$	0	0	0	0	0	0	0	$\frac{1}{14}$	0	0
	$\langle 232^23\rangle$	$\frac{1}{4}$	$\frac{1}{6}$	$\frac{1}{12}$	0	0	0	0	0	0	0	$\frac{1}{12}$	0	0	0	0	0
	$\langle 2323^2\rangle$	$\frac{2}{13}$	$\frac{2}{13}$	0	$\frac{1}{13}$	0	0	0	0	0	0	0	0	$\frac{1}{13}$	0	0	0
	$\langle 2^23^4\rangle$	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$	0	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$	0	0	0	$\frac{1}{16}$	0	$\frac{1}{16}$	0	$\frac{1}{16}$
	$\langle 2^43^2\rangle$	$\frac{2}{7}$	$\frac{1}{14}$	$\frac{1}{14}$	$\frac{1}{14}$	$\frac{1}{14}$	0	$\frac{1}{14}$	$\frac{1}{14}$	$\frac{1}{14}$	$\frac{1}{14}$	0	0	0	0	$\frac{1}{14}$	0
	$\langle 2^43^4\rangle$	$\frac{1}{5}$	$\frac{1}{20}$	$\frac{1}{20}$	$\frac{1}{20}$	$\frac{1}{20}$	$\frac{1}{20}$	$\frac{1}{20}$	$\frac{1}{20}$	$\frac{1}{20}$	$\frac{1}{20}$	0	$\frac{1}{20}$	0	$\frac{1}{20}$	$\frac{1}{20}$	$\frac{1}{20}$
	$\langle 2^43^3\rangle$	$\frac{4}{17}$	$\frac{1}{17}$	$\frac{1}{17}$	$\frac{1}{17}$	$\frac{1}{17}$	$\frac{1}{17}$	$\frac{1}{17}$	$\frac{1}{17}$	$\frac{1}{17}$	$\frac{1}{17}$	0	$\frac{1}{17}$	0	0	$\frac{1}{17}$	$\frac{1}{17}$
	$\langle 2^33^4\rangle$	$\frac{1}{6}$	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{18}$	0	$\frac{1}{18}$	0	$\frac{1}{18}$	0	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{18}$

† Note in order n_0 all vertices for orders $n_0' < n_0$ also occur, but their structural coefficients can be calculated easily and are hence not listed.

is certainly negative (for small w), so one concludes that $\langle 233\rangle$ *cannot* appear as a new stable phase between $\langle 3\rangle$ and $\langle 23\rangle$. As in the earlier discussion of the $\langle\infty\rangle\langle 3\rangle$ boundary, one anticipates that the $\langle 3\rangle$ and $\langle 23\rangle$ phases are separated by a first-order transition at $\delta = \delta_2(T) \approx \delta_2^{(2)}(T)$; this is borne out by the calculation of a positive interfacial tension between the phases (see §13). Finally, by a slightly more subtle argument (see lemma 2 below and subsequent analysis) one checks that $\langle 2233\rangle$ also cannot appear as an equilibrium phase.

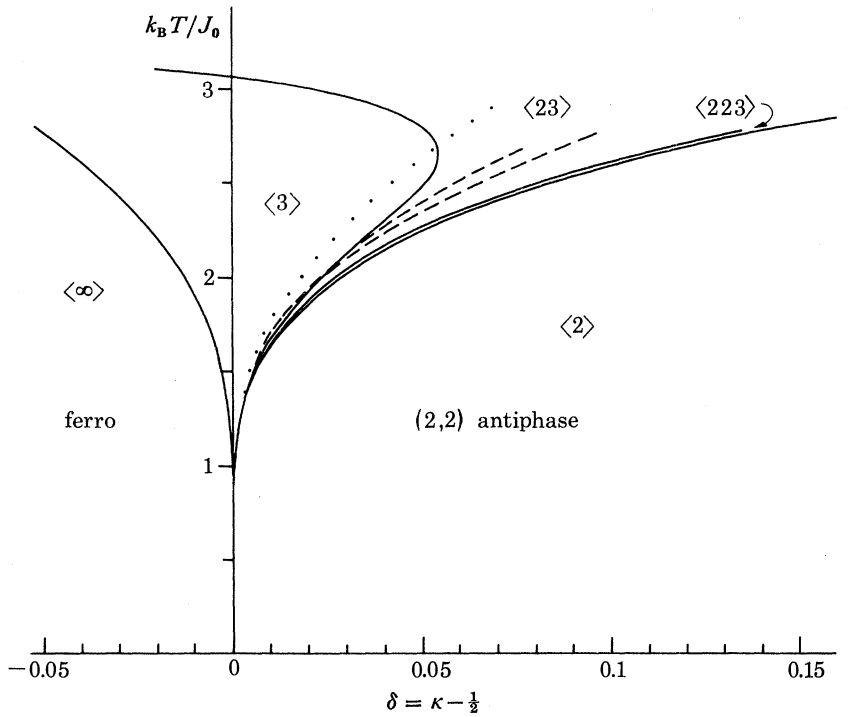

FIGURE 5. Phase boundaries in third order (solid curves) separating ferromagnetic (or $\langle\infty\rangle$), $\langle 3\rangle$, $\langle 23\rangle$, $\langle 223\rangle$, and $\langle 2\rangle$ phases. In higher order, extra phases $\langle 2^k 3\rangle$ appear between $\langle 223\rangle$ and $\langle 2\rangle$ phases, but of very narrow extent: see §§13 and 14. The dashed curves represent the $\langle 3\rangle\langle 23\rangle$ and $\langle 23\rangle\langle 2\rangle$ boundaries in second order, while the dotted curve represents the $\langle 3\rangle\langle 2\rangle$ boundary in first order. As demonstrated in §12, all boundaries of the form $\langle 2^k 3\rangle\langle 2\rangle$ are unstable or pseudo-phase boundaries while those between phases $\langle 2^{k-1}3\rangle$ and $\langle 2^k 3\rangle$ represent true first-order phase transitions.

The remaining boundaries to third order, $\delta_1^{(3)}$ between $\langle 3\rangle$ and $\langle 23\rangle$, $\delta_2^{(3)}$ between $\langle 23\rangle$ and $\langle 223\rangle$, and $\delta_3^{(3)}$ between $\langle 223\rangle$ and $\langle 2\rangle$, may be calculated by equating the full expansions for the free energies $f_{\langle 3\rangle}, f_{\langle 23\rangle}$, etc. (to third order) and solving the resulting nonlinear equations for δ (at fixed T) numerically. In figure 5 results for the case $J_0 = J_1$ on the simple cubic lattice are shown. In fact, the locus $\delta_3^{(3)}(T)$ seems to give a reasonably good numerical estimate of the true limiting stability boundary, $\delta_\infty(T)$, of the $\langle 2\rangle$ phase (see below) because for $\delta \lesssim 0.1$ the width of the $\langle 223\rangle$ phase region is already very small compared with the $\langle 23\rangle$ region and, as will be shown, the contribution of each higher-order phase decreases exponentially. Thus for $\delta = 0.1$ (or $\kappa = 0.6$) we conclude that the $\langle 2\rangle$ phase 'melts' at $k_B T \simeq 2.6 J_0/k_B$. This is about 10% lower than found in the Monte Carlo simulations (Selke & Fisher 1979, 1980*a*). The error in the latter is probably a result of the finite lattice used and the periodic boundary conditions with consequent wavevector quantization, which causes all transitions to appear discontinuous. The domain wall theory developed by Bak & von Boehm (1980) also gives an

overestimate, suggesting melting at $k_B T \simeq 2.85 J_0$. An interesting aspect of figure 5 is that the $\langle 3\rangle\langle 23\rangle$ boundary bends back towards negative δ. Although this result has been obtained by calculations limited to third order, we believe it is probably at least qualitatively correct. It is also plausible that higher-order calculations would reveal a similar 'peeling off' at larger values of δ (although, perhaps, without any bending back) of the higher-order boundaries such as $\langle 23\rangle\langle 223\rangle$. However, this raises the questions of the behaviour of the model at intermediate temperatures below the ultimate transition to the paramagnetic disordered state, of the existence of a floating or truly incommensurate phase, etc., which problems are beyond the scope of the present analysis.

As a further check on the nature of the phase diagram at intermediate temperatures as predicted in third order, the truncated expansions were studied numerically for the s.c. lattice with $J_0 = J_1$ in the region $\frac{1}{4} < \kappa < 1$, $k_B T/J_1 \leqslant 4.7$. No new phases are found in this order. In particular the phases $\langle 233\rangle$ and $\langle 2233\rangle$ are nowhere stable, in agreement with figure 5. Precisely *on* the $\langle 23\rangle\langle 223\rangle$ boundary all phases like $\langle 23223\rangle$, $\langle 2323223\rangle$, ..., $\langle (23)^j (223)^k\rangle$, $\langle (23)^j (223)^k (23)^{j'} (223)^{k'}\rangle$, etc. are stable in third order but, as proved below, all these phases are unstable in fifth order and so do not appear.

10. The structural spaces

In §8 we introduced the structural variables, l_μ, appropriate to discussing the 2:3 phases of ANNNI models which arise at low temperatures in the vicinity of $\kappa = \frac{1}{2}$ (or $\delta = 0$). The role played by these variables in elucidating the equilibrium phases was demonstrated by the explicit calculations presented in the previous section, where the structural spaces, $\mathscr{L}_n$, were introduced informally and exhibited for $n = 2$ and 3 in figures 3 and 4. Here we take up the development more systematically so as to lay a groundwork for the analysis of the equilibrium phases to all orders in the low temperature expansions.

The coordinates of the linear *structural space*, $\mathscr{L}_n$, of order n are constituted by the set of *standard structural variables*, l_ν (defined in §8), satisfying $n_0(\nu) \leqslant n$, where $n_0(\nu)$ is the span of the structural sequence ν. (Recall that the span is given explicitly in (8.13). The span requirement arises because, as seen in §9, the terms of order w^{nq_+} in the low temperature expansion cannot require knowledge of sequences ν of span exceeding n.) Points in $\mathscr{L}_n$ will be denoted $\boldsymbol{l}^{(n)}$, $\boldsymbol{u}^{(n)}$, and $\boldsymbol{v}^{(n)}$; the standard components of, for example, $\boldsymbol{u}^{(n)}$ will be the set $\{u_\nu^{(n)}\} \equiv \{l_\nu(\boldsymbol{u}^{(n)})\}$. The structural relations (8.4) can thus be rewritten as

$$l_\mu(\boldsymbol{u}^{(n)}) = \sum_\nu^{\leqslant} c_{\mu\nu} l_\nu(\boldsymbol{u}^{(n)}), \tag{10.1}$$

where the restricted sum runs only over the ν satisfying $n_0(\nu) \leqslant n$, while the $c_{\mu\nu}$ are independent of n.

Now a point $\boldsymbol{u}^{(n)}$ in $\mathscr{L}_n$ can be projected onto a lower-order space, $\mathscr{L}_{n^-}$, with $n^- < n$, in the obvious way by setting $l_\nu(\boldsymbol{u}^{(n)}) = 0$ for $n_0(\nu) > n^-$. The general 2:3 structures can be specified by the set of all standard variables $\{l_\nu\}$, where the lengths, $m(\nu)$, and spans, $n_0(\nu)$, extend up to infinity. Hence we introduce the complete structural space $\mathscr{L} \equiv \mathscr{L}_\infty$, with points $\boldsymbol{l} = \boldsymbol{l}^{(\infty)}$, $\boldsymbol{u} = \boldsymbol{u}^{(\infty)}$, $\boldsymbol{v} = \boldsymbol{v}^{(\infty)}$. Definite structures of the lattice layers may be identified with corresponding points $\boldsymbol{u}$, and we may use the phrase 'the structure $\boldsymbol{u}$'. Such structural points can be projected down into $\mathscr{L}_n$.

The dimension $D_n = \dim[\mathscr{L}_n]$, of $\mathscr{L}_n$ is clearly just the number of standard structural sequences ν satisfying $n_0(\nu) \leqslant n$. One finds from the listing (8.16)–(8.19), of the standard sequences ν, the values

$$D_n = 1, 2, 4, 7, 12, 21, 37, \tag{10.2}$$

for $n = 1, 2, \ldots, 7$. An exact expression for general n is

$$\begin{aligned} D_n &= D_{n-1} + \sum_{j=1}^{\frac{1}{3}(n+1)} \binom{n-j}{2j-1} \\ &= 1 + \sum_{m=2}^{n} \sum_{j=1}^{\frac{1}{3}(m+1)} \binom{m-j}{2j-1}, \end{aligned} \tag{10.3}$$

where, in fact, rather few terms in the sums are non-zero for modest n. For large n the asymptotic behaviour is

$$D_n \approx A\xi_0^n, \tag{10.4}$$

where $\xi_0 \approx 1.754\,877\,666$ is the real root of $\xi^3 - 2\xi^2 + \xi - 1 = 0$ and $A \simeq 0.721$ (which may be expressed explicitly in terms of ξ_0). Actually, one has $D_n = \{A\xi_0^n\}'$, where $\{x\}'$ denotes the integer closest to x. From the bounds $m(\mu) \leqslant n_0(\mu) \leqslant \frac{3}{2}m(\mu) - 1$ (see §8), and the fact that there are 2^{m_0-2} standard sequences of length $m(\nu) = m_0$ we find

$$2^{\frac{2}{3}n-\frac{1}{3}} \leqslant D_n \leqslant 2^n \quad (n \geqslant 2), \tag{10.5}$$

in agreement with the exact results. Evidently the dimensions of the $\mathscr{L}_n$ increase rapidly with n, but, happily, we will be able to confine attention, at stage n, to rather small subspaces. One may introduce a norm $\|\boldsymbol{u}\|$ for a general structure $\boldsymbol{u}$, a convenient choice being

$$\|\boldsymbol{u}\| = \{\sum_{\nu} 2^{-n_0(\nu)}[l_\nu(\boldsymbol{u})]^2\}^{\frac{1}{2}}, \tag{10.6}$$

although the exact form will play no special role. (One may replace 2 by any number exceeding ξ_0.) If $\boldsymbol{u} \equiv \boldsymbol{u}^{(n)}$ is specified only to order n, the sum should be appropriately truncated.

A class of important general structures already stressed are the periodic structures $\langle\mu\rangle$, defined (for all $m \leqslant \infty$) as generated from the structural sequence μ by periodic repetition to obtain a full, infinite lattice structure. If, initially, $\boldsymbol{u}^{(n)}$ arises by projection of $\langle\mu\rangle$ on to $\mathscr{L}_n$, we may, conversely, *extend* $\boldsymbol{u}^{(n)}$ to all $\boldsymbol{u}^{(n^+)}$, where $n^+ > n$, by the obvious prescription. If μ has $m_2 + m_3 = m(\mu)$ bands (m_2 2-bands and m_3 3-bands) which alternate 'up–down' in the corresponding ground state, then the spin pattern repeats in, at least, a length of $2(2m_2 + 3m_3)$ lattice layers, and that length includes precisely m 'up–down' sequences. Hence the (mean) wavelength is

$$\lambda = \frac{2(2m_2 + 3m_3)\,a}{m} = 4\left(1 + \frac{m_3}{2m}\right) a = \frac{2\pi}{\bar{q}},$$

where $\bar{q} \equiv |\boldsymbol{q}|$ is the (mean) wavenumber. The same wavelengths and wavenumbers apply to the ground states and to the thermodynamic equilibrium states based on the periodic ground states specified by $\langle\mu\rangle$. For the special states $\langle 2^{j-1}3\rangle$, with $j = 1, 2, \ldots$ (where $j = 1$ corresponds to $\langle 3\rangle$) we have the wavenumbers

$$\bar{q} \equiv \bar{q}_j = \pi j/(2j+1)\,a. \tag{10.7}$$

Obviously, there are points $\boldsymbol{u}^{(n)}$, in the space $\mathscr{L}_n$, that do not correspond to any consistent or *realizable structure* of the lattice, e.g. any point with $l_2(\boldsymbol{u}^{(n)}) = 0$, but $l_{23}(\boldsymbol{u}^{(n)}) > 0$. We state this fact in a formal way: *if* $\boldsymbol{u}^{(n)}$ *corresponds to a realizable structure, then there exists at least one full,*

infinite lattice structure, that determines a set $\{l_\nu^0\}$ *for* $n_0(\nu) \leqslant n$ *such that* $l_\nu(\boldsymbol{u}^{(n)}) = l_\nu^0$. For example, the periodic structures ($\langle\mu\rangle \equiv \boldsymbol{u}$) are certainly realizable. Also, any convex combination of a set, $\{\boldsymbol{u}_j^{(n)}\}$, of periodic structures

$$\boldsymbol{l}^{(n)} = \sum_{j=1}^{k} \theta_j \boldsymbol{u}_j^{(n)} \quad \text{with} \quad \sum_{j=1}^{k} \theta_j = 1, \quad \theta_j \geqslant 0, \tag{10.8}$$

is realizable: merely consider a structure where $\theta_1 L$ layers of the finite periodic structure $\boldsymbol{u}_1$ are followed by $\theta_2 L$ layers of the type $\boldsymbol{u}_2$, etc. and $L \to \infty$. For any realizable structure, $\boldsymbol{u}^{(n)}$, one clearly has

$$l_\mu(\boldsymbol{u}^{(n)}) \geqslant 0, \quad \text{for all } \mu \text{ with } \quad n_0(\mu) \leqslant n. \tag{10.9}$$

This represents a set of

$$I_n = 3D_n - 1 \tag{10.10}$$

linear inequalities, since for each of the D_n cores for $m(\mu) \geqslant 2$ there are three distinct inequalities (see (8.2) and (8.3)), whereas there are only two for $m(\mu) = 1$. The realizable points $\boldsymbol{u}^{(n)}$ are thus confined to a convex *structural polytope* $\mathscr{P}_n$, as illustrated in figures 3 and 4. The vertices of the structural polytope will be denoted $\boldsymbol{v}_j^{(n)}$ with $j = 0, 1, 2, \ldots$ and $j_{\max} \geqslant D_n$. The *edges* will be labelled by $\boldsymbol{e} \equiv (\boldsymbol{v}_i^{(n)}, \boldsymbol{v}_j^{(n)})$, the plane faces by $(\boldsymbol{v}_i^{(n)}, \boldsymbol{v}_j^{(n)}, \boldsymbol{v}_k^{(n)})$, etc. As illustrated in figure 3 and discussed in §8, the complete set of vertices $\{\boldsymbol{v}_j^{(n)}\}$ in order n can be found from the inequalities (10.9) either by exhaustive algebraic analysis or, numerically, by exploration with the use of linear programming algorithms (see, for example, Wilf 1962, Gass 1964). In the leading orders one finds (see table 4) that all vertices $\boldsymbol{v}_j^{(n)}$ correspond to unique periodic structures (up to a trivial axial translation). These vertices can thus be labelled $\langle\mu\rangle$ and extend naturally to all n. We will, in fact, prove that all vertices that correspond to equilibrium states are, in fact, realizable only as unique periodic structures of the type $\langle 2^{j-1}3\rangle$ with j an integer.

11. Structural expansion and sequential calculation

The analysis presented in §§3, 4, 7, and 9 of the low temperature expansion in powers of w about a ground state specified by structural variables l_μ establishes that the reduced free energy per spin, in the vicinity of $\kappa = \frac{1}{2}$ (or $\delta = 0$), may be written

$$f(w, x; \delta; \{l_\mu\}) = a_0(w, x; \delta) + \sum_\nu a_\nu(w, x; \delta)\, l_\nu, \tag{11.1}$$

where the sum runs over all standard structural variables (see (9.11)). Furthermore, because a connected configuration of n overturned spins has a maximum span we also have

$$a_\nu(w, x; \delta) = w^{q_\perp n_0(\nu)} b_\nu(w, x; \delta), \tag{11.2}$$

for $n_0(\nu) \geqslant 2$, with

$$b_\nu(w, x; \delta) = b_\nu^{(0)}(x; \delta)\,[1 + O(w^{q_\perp - 2})], \tag{11.3}$$

where $b_\nu^{(0)}(x; \delta)$ is a 'polynomial' in x and x^δ in which some negative powers of x^δ may appear, while the leading term in the correction factor arises from configurations with two overturned spins adjacent in the same layer (see (9.13) and the explicit calculations presented in §9 and tables 1, 2, and 3). This result enables the structural expansion (11.1) to be studied systematically in successive powers of, essentially, $w^{q_\perp}$. Our basic assumption is that the convergence for small w is sufficiently good that the equilibrium phases can be found by minimizing the free energy (or, maximizing, $f\{l_\mu\}$) order-by-order, over the variables $\boldsymbol{l} \equiv \{l_\mu\}$ representing all

realizable structures. The allowable $\boldsymbol{l}$ are contained in the infinite-dimensional polytope, $\mathscr{P} \equiv \mathscr{P}_\infty$, in $\mathscr{L}$. We can thus write for the true, equilibrium free energy of the model

$$f_{\mathrm{eq}}(w, x; \delta) = a_0(w, x; \delta) + \max_{\boldsymbol{l} \in \mathscr{P}_\infty} \{\Delta f(\boldsymbol{l}; \delta)\}, \tag{11.4}$$

where a_0 follows from (4.6) or (9.7) and (9.8), while

$$\Delta f(\boldsymbol{l}; \delta) = a_2(w, x; \delta)\, l_2 + \sum_{n=2} w^{nq_\perp} \sum_{\nu}^{(n)} b_\nu(w, x; \delta)\, l_\nu, \tag{11.5}$$

where the restricted sum runs over ν of span $n_0(\nu) = n$. Note that, on reproducing (4.7), we have

$$a_2(w, x; \delta) = \tfrac{4}{3}K_1\,\delta - \tfrac{2}{3}(2 - 3x^{1+2\delta} + x^{3+2\delta})\, w^{q_\perp} + O(w^{2q_\perp - 2}), \tag{11.6}$$

(see also (9.7) and (9.8) and tables 2 and 3); the significant feature here is that a_2 has a 'strong' (w-independent) linear variation with δ.

Evidently $\Delta f(\boldsymbol{l}; \delta)$ is a linear function of $\boldsymbol{l}$ and its maxima are required subject to the linear constraints (10.9) (with (10.1)) which determine the structural polytope $\mathscr{P}_\infty$. As remarked before, this specifies a problem in linear programming – strictly of infinite order. Now the solution of a linear programming problem is generically unique and corresponds to a single vertex, the maximal vertex, of the polytope $\mathscr{P}$ specified by the constraints (see e.g. Wilf 1962, Gass 1964). Here and below we consider fixed T, i.e. fixed x and w, but varying δ. Then as δ changes, the $a_\nu(\delta)$ or $b_\nu(\delta)$ vary continuously but the maximal vertex $\boldsymbol{v}(\delta)$ can only change discontinuously. *At* such a discontinuity or transition point (or boundary), say $\delta = \delta_\sigma$, there will, by the results of linear programming theory, be, in general, a unique extremal edge, $\boldsymbol{e}_\sigma$, of $\mathscr{P}$ joining the two maximal vertices $\boldsymbol{v}(\delta_\sigma^+)$ and $\boldsymbol{v}(\delta_\sigma^-)$. It may be anticipated that as δ passes through δ_σ a first-order thermodynamic transition occurs: however, this needs verification by the exhibition of a discontinuity in one or more of the first derivatives of $f_{\mathrm{eq}}(w, x; \delta)$ at $\delta = \delta_\sigma$ or, by evaluation, of a positive surface tension, Σ_σ, between the phases, which can coexist at $\delta = \delta_\sigma$. Of course, insofar as $\boldsymbol{v}(\delta_\sigma^+)$ and $\boldsymbol{v}(\delta_\sigma^-)$ determine distinct ground state structures and hence distinct long-range-order parameters, the first-order character of the transition is certainly to be expected (see §13).†

To calculate the maximal vertices explicitly we will use the sequential nesting of the structural spaces, $\mathscr{L}_1 \subset \mathscr{L}_2 \subset \ldots \subset \mathscr{L}_\infty$, associated with the powers of $w^{q_\perp}$ through equation (11.5). Thus at stage n we determine the sequence of maximal vertices $\boldsymbol{v}_j^{(n)}$ ($j = 0, 1, 2, \ldots$) and the transition boundaries, say $\delta = \delta_j^{(n)}$, between $\boldsymbol{v}_j$ and $\boldsymbol{v}_{j-1}$. The boundaries and free energies can be found explicitly up to corrections of order $w^{(n+1)q_\perp}$. We take

$$\delta_1^{(n)} < \delta_2^{(n)} < \ldots < \delta_j^{(n)} < \ldots . \tag{11.7}$$

(The consistency with the notation used in §9 will emerge.) Note that the transition boundary $\delta_j^{(n)}$ is defined explicitly by

$$\Delta f(\boldsymbol{v}_j^{(n)}; \delta_j^{(n)}) = \Delta f(\boldsymbol{v}_{j-1}^{(n)}; \delta_j^{(n)}) + O(w^{(n+1)q_\perp}). \tag{11.8}$$

Now take $\epsilon > 0$ (fixed as $w \to 0$) and consider the interval

$$\delta_j^{(n)} < \delta < \delta_{j+1}^{(n)}, \tag{11.9}$$

† It is appropriate here to mention that Kudo & Katsura (1976) have used the linear programming procedure sketched here to study the ground state orderings of various Ising models with several neighbour interactions in a magnetic field.

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corresponding to the *stability* (or maximality) of the vertex $\boldsymbol{v}_j^{(n)}$. For δ in this interval the free energy $\Delta f(\boldsymbol{v}_j^{(n)};\, \delta)$ exceeds $\Delta f(\boldsymbol{u}^{(n)})$ for all $\boldsymbol{u}^{(n)}$ in $\mathscr{P}_n$ not equal to $\boldsymbol{v}_j^{(n)}$ by terms of order at least $w^{nq_\perp}$ provided

$$\|\boldsymbol{u}^{(n)} - \boldsymbol{v}_j^{(n)}\| = \epsilon > 0. \tag{11.10}$$

Addition of higher-order terms, $n+1, n+2, \ldots$ to the full free energy expressions in $\mathscr{P}_{n+1}$, $\mathscr{P}_{n+2}, \ldots$ cannot alter this for sufficiently small w, since the sum of terms of order $w^{(n+1)q_\perp}$ cannot overwhelm terms of order $w^{nq_\perp}$ (assuming, as stated, sufficiently good convergence of the series).

Explicitly, subject to (11.8) *and* (11.9), one concludes

$$\Delta f(\boldsymbol{v}_j^{(n)};\, \delta) \geqslant \Delta f(\boldsymbol{u};\, \delta) + A_n\, \epsilon w^{nq_\perp}, \tag{11.11}$$

for all $\boldsymbol{u} \in \mathscr{P}_\infty$, where $A_n > 0$ can be found independently of $\boldsymbol{u}$, even though (11.10) applies only with $\boldsymbol{u}^{(n)}$, the projection of $\boldsymbol{u}$ on to $\mathscr{P}_n$.

Note, however, that for δ in the *vicinity of the boundary* $\delta_j^{(n)}$, in the sense

$$\delta = \delta_j^{(n)} + O(w^{(n+1)q_\perp}), \tag{11.12}$$

one must consider the vicinity of the line

$$\boldsymbol{e}_j^{(n)}(\theta) \equiv \boldsymbol{l} = \theta \boldsymbol{v}_j^{(n)} + (1-\theta)\, \boldsymbol{v}_{j-1}^{(n)}, \tag{11.13}$$

with $0 \leqslant \theta \leqslant 1$, i.e. of the *maximal edge* joining the transition vertices. For this, by the same reasoning, one has

$$\Delta f(\boldsymbol{u};\, \delta) \leqslant \Delta f(\boldsymbol{e}_j^{(n)};\, \delta) - B_n\, \epsilon w^{nq_\perp}, \tag{11.14}$$

for all $\boldsymbol{u} \in \mathscr{P}_\infty$, where $\epsilon = \min_\theta \|\boldsymbol{u}^{(n)} - \boldsymbol{e}_j^{(n)}(\theta)\|$. Note, nonetheless, that if the projection $\boldsymbol{u}^{(n)}$ lies *on* the edge $\boldsymbol{e}_j^{(n)}$ one may have $\Delta f(\boldsymbol{u};\, \delta)$ exceeding $\Delta f(\boldsymbol{e}_j^{(n)})$ in higher order: this allows for the instability of a transition of order n and the appearance of a new, interpolating phase, in higher order (as illustrated explicitly in the computations of § 9).

Now consider the effects of terms in the structural expansion (11.5) of order $n+1$, i.e. magnitude $O(w^{(n+1)q_\perp})$. At this stage there are just two alternatives: the *basic dichotomy*. *Either* (*a*) for δ in the vicinity of $\delta_j^{(n)}$ one or more new maximal (higher-order) vertices appear; then the analysis must recommence about the boundaries between these vertices; *or* (*b*) one may find that the vertices $\boldsymbol{v}_j^{(n)}$ and $\boldsymbol{v}_{j-1}^{(n)}$ *extend* (see previous section) as maximal vertices to (effectively) the same vertices $\boldsymbol{v}_{j_+}^{(n)}$ and $\boldsymbol{v}_{j_+-1}^{(n)}$ (where j_+ is the appropriate new label in the new, $(n+1)$-stage sequential labelling of the vertices) and the maximal edge $\boldsymbol{e}_{j_+}^{(n+1)}$ (see (11.13)) remains maximal on the extended transition boundary

$$\delta = \delta_{j_+}^{(n+1)} = \delta_j^{(n)} + O(w^{(n+1)q_\perp}). \tag{11.15}$$

This means that for δ in the range $(\delta_{j_+-1}^{(n+1)} + \eta,\ \delta_{j_++1}^{(n+1)} - \eta)$ for some $\eta > 0$, one has

$$\Delta f(\boldsymbol{e}_{j_+}^{(n+1)}(\theta);\, \delta) \geqslant \Delta f(\boldsymbol{u};\, \delta) + B_{n+1}\, \epsilon w^{(n+1)q_\perp}, \tag{11.16}$$

for any $\boldsymbol{u}$ in $\mathscr{P}$ with $\|\boldsymbol{u} - \boldsymbol{e}_{j_+}^{(n+1)}(\theta)\| > \epsilon > 0$. In case (*b*) we thus conclude that $\boldsymbol{v}_j^{(n)}$ and $\boldsymbol{v}_{j-1}^{(n)}$, appropriately extended, remain extremal to all orders and that *there exists a true phase transition boundary* $\delta = \delta_{j_\infty}^{(\infty)}$, in the vicinity of $\delta_j^{(n)}$. Evidently, in case (*b*) the analysis of the general structure of the phase diagram in the vicinity of $\delta_j^{(n)}$ terminates at the stage $n+1$.

It seems clear intuitively that in proceeding to examine the vicinity of $\delta_j^{(n)}$ in stage $n+1$ it should not be necessary to study the whole polytope $\mathscr{P}_{n+1}$; rather it should suffice to evaluate

structural coefficients and so on, only for some vicinity of the edge $\boldsymbol{e}_{j_+}^{(n+1)}$. To make this precise, we state a lemma which helps delineate such 'feasible' structures, $\boldsymbol{u}$:

LEMMA 2: LOCALIZATION. *For* $\delta = \delta_j^{(n)} + O(w^{(n+1)q_\perp})$ *only the subspaces* $\mathscr{P}_{j,n+p}$ *of* $\mathscr{P}_{n+p}$ $(p = 1, 2, \ldots)$ *spanned by* $\boldsymbol{u}$ *which are consistent with at least one of the maximal vertices* $\boldsymbol{v}_j^{(n)}$ *and* $\boldsymbol{v}_{j-1}^{(n)}$ *(in order* n*) need be considered in searching for new maximal vertices.*

Before proving this lemma we must define 'consistency': a structure $\boldsymbol{u}$ is *consistent* with a set of structures $\{\boldsymbol{v}_i\}$ in nth order if there is no structural sequence μ with $n_0(\mu) \leqslant n$ such that $l_\mu(\boldsymbol{u}) > 0$ but $l_\mu(\boldsymbol{v}_i) = 0$ for all i. If such a μ exists, $\boldsymbol{u}$ is *inconsistent* with $\{\boldsymbol{v}_i\}$. To understand this, note that $l_\mu(\boldsymbol{v})$ measures the number of structural sequences μ implied by the structure $\boldsymbol{v}$. If $l_\mu(\boldsymbol{v}) = 0$, then any structure implying μ is inconsistent with $\boldsymbol{v}$. Consider for example the structures

$$\boldsymbol{v} = \theta\langle 23\rangle + (1-\theta)\langle 2\rangle \quad (0 \leqslant \theta \leqslant 1), \tag{11.17}$$

at some stage $n > 2$. Then $l_{33}(\boldsymbol{v}) = 0$ for all θ, as can be seen from table 4 and the structural relation (8.6), namely $l_{33} = \frac{1}{3} - \frac{2}{3}l_2 - l_{23}$. But consider $\boldsymbol{u} = \langle 233\rangle$ for which $l_{33}(\boldsymbol{u}) = \frac{1}{8} > 0$. Thus $\boldsymbol{u}$ is inconsistent with $\boldsymbol{v}$ and especially, putting $\theta = 0$ and 1, with the pair $(\langle 23\rangle, \langle 2\rangle)$. Conversely, take $\boldsymbol{u} = \langle 223\rangle$: by checking all the sequences with $n_0(\mu) \leqslant 2$, namely 2, 3, 22, 23, 32, and 33, one finds that this $\boldsymbol{u}$ *is* consistent with the pair $(\langle 23\rangle, \langle 2\rangle)$.

Proof of lemma 2. Consider some structure $\boldsymbol{u}$, actually realizable, which is a candidate for a maximal vertex in the vicinity of $\delta_j^{(n)}$ at some stage exceeding n and suppose $\boldsymbol{u}$ is *not* consistent with the pair $(\boldsymbol{v}_j^{(n)}, \boldsymbol{v}_{j-1}^{(n)})$. Then, by definition, there is a structural sequence μ of span $n_0(\mu) \leqslant n$, such that $l_\mu(\boldsymbol{u}) > 0$ while

$$l_\mu(\boldsymbol{v}_j^{(n)}) = 0 \quad \text{and} \quad l_\mu(\boldsymbol{v}_{j-1}^{(n)}) = 0. \tag{11.18}$$

From this relation and the definition of (11.13) of the edge $\boldsymbol{e}_j^{(n)}$ we have

$$l_\mu[\boldsymbol{e}_j(\theta)] = 0, \quad \text{for all} \quad 0 \leqslant \theta \leqslant 1. \tag{11.19}$$

Note that if $\boldsymbol{u}^{(n)}$ is the projection of $\boldsymbol{u}$ on to $\mathscr{P}_n$ the structural relations (10.1) imply

$$l_\mu(\boldsymbol{u}^{(n)}) = l_\mu(\boldsymbol{u}) > 0. \tag{11.20}$$

It follows that $\boldsymbol{u}^{(n)}$ cannot lie on the edge $\boldsymbol{e}_j^{(n)}$. But then, by (11.14), for δ in the vicinity of $\delta_j^{(n)}$ one has

$$\begin{aligned} \Delta f(\boldsymbol{u}) &= \Delta f(\boldsymbol{u}^{(n)}) + O(w^{(n+1)q_\perp}) \\ &\leqslant \theta \Delta f(\boldsymbol{v}_j^{(n)}) + (1-\theta)\,\Delta f(\boldsymbol{v}_{j-1}^{(n)}) - B_n \epsilon w^{nq_\perp}, \end{aligned} \tag{11.21}$$

where $\epsilon = \min_\theta \|\boldsymbol{u}^{(n)} - \boldsymbol{e}_j(\theta)\|$. Hence $\boldsymbol{u}$ cannot be a maximal vertex in any order n or greater (although it *could* be maximal in some lower order). This proves the lemma.

We will apply this lemma specifically to establish two basic propositions concerning the transition boundaries between $\langle 2^k 3\rangle$ and $\langle 2\rangle$ and between $\langle 2^k 3\rangle$ and $\langle 2^{k-1}3\rangle$. Note, however, that we still have to establish that these structures appear as maximal vertices at a general stage; this will be done in the next section where the sequence of phases is discussed.

Consider first the *transition boundary*, $\delta = \delta_{k+1}^{(k+1)}$, *between structures* $\boldsymbol{v}_k = \langle 2^k 3\rangle$ *and* $\boldsymbol{v}_\infty = \langle 2\rangle$ for $k = 0, 1, 2, \ldots$, *defined in order* $n = k+1$. We will examine all standard substructures ν of order $n+1$ or length $m(\nu) = k+2$ by considering all 2^k cores $\tilde{\nu}$ of length k and testing for inconsistency with $\boldsymbol{v}_k$ and $\boldsymbol{v}_\infty$ by taking into account all structures $\boldsymbol{u}$ for which $l_\nu(\boldsymbol{u}) > 0$. The cores $\tilde{\nu}$ may be classified by the number of 3-bands they contain as follows:

(i) Zero 3-bands, so $\tilde{\nu} = 2^k$. In the case, by the standard convention (see §8), one has

$\nu = 2^{k+1}3$. No proof of inconsistency of $\boldsymbol{u}$ for which $l_{2^{k+1}3}(\boldsymbol{u}) > 0$ will be presented. Indeed, it transpires that none can be given!

(ii) One 3-band or $\tilde{\nu} = 2^j 32^{k-1-j}$ with $0 \leqslant j \leqslant k-1$. Then by convention A (§8) one gets $\nu = \nu_{\mathrm{A}} = 2^{j+1}32^{k-1-j}3$, provided, to avoid subperiodicity, one has (A) $j+1 > k-1-j$. Otherwise, (B), one must use convention B, so that $\nu = \nu_{\mathrm{B}} = 32^j 32^{k-j}$ for $j+1 \leqslant k-1-j$. Consider case (A): we know from lemma 1 (§8) that $l_{\nu_-}(\boldsymbol{u}) > 0$, if $l_\nu(\boldsymbol{u}) > 0$ and ν_- is any subsequence of ν. Thus choose $\nu_- = 32^{k-1-j}3$. By direct inspection of the periodic structures $\langle 2^k 3\rangle$ and $\langle 2\rangle$ one finds $l_{\nu_-}(\boldsymbol{v}_k) = l_{\nu_-}(\boldsymbol{v}_\infty) = 0$ for any $j \geqslant 0$. Hence any postulated $\boldsymbol{u}$ with $l_\nu(\boldsymbol{u}) > 0$ is not consistent with the pair $(\boldsymbol{v}_k, \boldsymbol{v}_\infty)$. In case (B) choose the subsequence $\nu_- = 32^j 3$, where $j \leqslant k-1$. By inspection, ν_- cannot arise in $\boldsymbol{v}_k$ or $\boldsymbol{v}_\infty$ and so, again, $\boldsymbol{u}$ with $l_{\nu_{\mathrm{B}}}(\boldsymbol{u}) > 0$ is not consistent.

(iii) Two or more 3-bands (e.g. $\tilde{\nu} = 2^i 32^j 32^{k-1-i-j}$). It suffices now to choose a substructure ν_- of both ν_{A} and ν_{B} (defined by the conventions A and B as in (ii)) containing at least two 3-bands, say $\nu_- = 32^j 3$, with, necessarily, $j < k$. Obviously such a subsequence cannot arise in $\boldsymbol{v}_k$ or $\boldsymbol{v}_\infty$. Thus if $l_{\nu_{\mathrm{A}}}(\boldsymbol{u})$ or $l_{\nu_{\mathrm{B}}}(\boldsymbol{u})$ are non-zero $\boldsymbol{u}$ is not consistent with $\boldsymbol{v}_k$ or $\boldsymbol{v}_\infty$.

We conclude that, in stage $n+1$, any $\boldsymbol{u} \in \mathscr{P}_{n+1}$ for which l_ν is non-zero for any standard configuration other than $\nu = 2^{k+1}3$, from case (i), is not consistent with $(\boldsymbol{v}_k, \boldsymbol{v}_\infty)$. Thus by lemma 2 we have:

PROPOSITION 1. *On the boundary $\langle 2^k 3\rangle$–$\langle 2\rangle$ in stage $n+1 = k+2 \geqslant 2$ it suffices to consider only general structures for which $l_{2^{k+1}3} \geqslant 0$ while $l_\nu = 0$ for all $\nu \neq 2^{k+1}3$ of order $m(\nu) = k+2$.* (In higher orders no other terms enter.) *In addition, the projection of any feasible $\boldsymbol{u}^{(k+2)}$ on to $\mathscr{P}_{k+2}$ must lie on the edge $\boldsymbol{e}_{k,\infty}(\theta) = \theta \boldsymbol{v}_k^{(n)} + (1-\theta)\boldsymbol{v}_\infty^{(n)}$ $(0 \leqslant \theta \leqslant 1)$, since otherwise Δf is no longer maximal, as shown.*

In a parallel manner we now analyse the transition boundary $\delta = \delta_k^{(k+1)}$ between the structures $\boldsymbol{v}_k = \langle 2^k 3\rangle$ and $\boldsymbol{v}_{k-1} = \langle 2^{k-1}3\rangle$ for $k = 1, 2, 3, \ldots$ at order $n = k+1$, assuming tacitly its relevance, which will be seen later. We examine all standard sequences ν of span $n_0(\nu) > k+1$. Again, the sequences may be classified by the number of 3-bands in the cores $\tilde{\nu}$:

(i) Zero 3-bands, so $\tilde{\nu} = 2^j$ $(j \geqslant k)$. Choose $\nu_- = 2^{j+1}$ so that one has $l_{\nu_-}(\boldsymbol{v}_k) = l_{\nu_-}(\boldsymbol{v}_{k-1}) = 0$ for $j \geqslant k$. Hence any $\boldsymbol{u}$ with $l_\nu(\boldsymbol{u}) > 0$ is not consistent with the pair $(\boldsymbol{v}_k, \boldsymbol{v}_{k-1})$.

(ii) One 3-band or $\tilde{\nu} = 2^i 32^j$ with $i+j+1 \geqslant k$, $i, j \geqslant 0$. Then, by convention A one has $\nu = \nu_{\mathrm{A}} = 2^{i+1}32^j 3$, provided (A) $i+1 > j$, to avoid subperiodicity; otherwise (B) one has $\nu = \nu_{\mathrm{B}} = 32^i 32^{j+1}$. In case (A) choose $\nu_- = 32^j 3$. This yields inconsistency unless either (*a*) $j = k$ or (*b*) $j = k-1$. If (*a*) holds, then choose $\nu_- = 2^{i+1}$ with $i+1 > j = k$; this yields inconsistency. If (*b*) holds, choose $\nu_- = 2^{i+1}$ with $i+1 \geqslant k$; this yields inconsistency for the inequality. Hence, the *only remaining case is* $i+1 = k$ *or* $\nu = 2^k 32^{k-1}3$ *at* $n_0(\nu) = 2k+1$. Case (B) yields inconsistency either with $\nu_- = 32^i 3$ or, for $i = k$ or $i = k-1$, with $\nu_- = 2^{j+1}$.

(iii) Two 3-bands or $\tilde{\nu} = 2^h 32^i 32^j$, with $h+i+j+2 \geqslant k$ and $h, i, j \geqslant 0$. (A) For $h+1 > j$, to avoid subperiodicity, convention A applies and one gets $\nu = \nu_{\mathrm{A}} = 2^{h+1}32^i 32^j 3$. Otherwise, (B) one has $\nu = \nu_{\mathrm{B}} = 32^h 32^i 32^{j+1}$. Now, in case (A) choosing $\nu_- = 32^i 3$ and $32^j 3$ yields $i, j = k, k-1$ as the only possibilities, which on excluding subperiodic sequences implies $h \geqslant k, k-1$. Hence, on computing the span $n_0(\nu) = 5+h+i+j \geqslant 3k+2 = n+(2n-1)$, the *lowest-order standard sequence not excluded is* $\nu = 2^k 32^{k-1}32^{k-1}3$ *at* $n_0 = n+(2n-1)$. Case (B) always yields inconsistency, as seen by first choosing $\nu_- = 32^k 3$ and $32^i 3$, and then, for $h, i = k, k-1$, choosing $\nu_- = 2^{j+1}$.

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(iv) Three and more 3-bands with $\tilde{\nu} = 2^{i_0}32^{i_1}3\ldots32^{i_g}$, where $g = \tilde{m}_3$ denotes the number of 3-bands. Convention A applies for $i_0 > i_g$ and $i_1, i_2, \ldots, i_g \geqslant k, k-1$. Again, standard sequences similar to those remaining in (iii) cannot be excluded. Their spans, however, satisfy $n_0 \geqslant n + [\tilde{m}_3(n-\frac{1}{2}) - \frac{1}{2}]$. When convention B applies, inconsistency is found in all cases.

Thus we have established:

PROPOSITION 2. *On the boundary* $\langle 2^{k-1}3\rangle$–$\langle 2^k3\rangle$ *in order* $n = k+1 \geqslant 2$ *it suffices to consider only structures* $\boldsymbol{u}$ *with* $l_\nu(\boldsymbol{u}) > 0$ *for* $\nu = 2^k32^{k-1}3$, *but* $l_\nu(\boldsymbol{u}) = 0$ *for all other* ν *at stage* $n+p$ *with* $p = n-1$. (At this stage such new structures, $\boldsymbol{u}$, do occur, and they represent the leading *possible* instability of the transition boundary $\delta_k^{(k+1)}$. Subsequent corrections arise only in stages $n+p'$ with $p' = 2n-1, 3n-2$, etc.). *Furthermore, the projection of any feasible* $\boldsymbol{u}^{(n+p)}$ *on to* $\mathscr{P}_n$ *must lie on the edge* $\boldsymbol{e}_{k\_}(\theta) = \theta\boldsymbol{v}_{k-1} + (1-\theta)\boldsymbol{v}_k$ $(0 \leqslant \theta \leqslant 1)$, *as before.*

Actually, the 'instability' turns out to be unrealized, as will be seen from the explicit calculations of the sequence of phases in the next section. However, the relevant structural sequences of order $2n-1$ do serve to establish that the transition is of first order and to aid in evaluation of the corresponding interfacial tension.

12. THE SEQUENCE OF PHASES

We now combine the previous analysis, the expression (11.6) for $a_2(w, x; \delta)$, and the two special results

$$b_{2^k3}(w, x; \delta) \approx (k+2)(1-x^2)(1-x^{1+2\delta})^{k+1}, \tag{12.1}$$

where the span is $n_0(2^k3) = (k+1)$, and

$$b_{2^k32^{k-1}3}(w, x; \delta) \approx -x^{1-2\delta}(1-x^{1+2\delta})^{2(k+1)}, \tag{12.2}$$

with span $n_0(2^k32^{k-1}3) = 2k+1$, which are both valid for $k = 1, 2, \ldots$, with correction factors $1 + O(w^{q_\perp - 2})$. This will enable us to establish the sequence of phases and phase transition boundaries. The crucial results (12.1) and (12.2) are derived in the Appendix. As previously, we take $x < 1$ fixed, and w fixed and sufficiently small. It follows that a_{2^k3} is positive but $a_{2^k32^{k-1}3}$ is *negative* for small T and δ. We proceed by analysing the low temperature expansion, order by order. The first few stages essentially duplicate the analysis of §9 but are presented for completeness.

(i) *First order.* For $n = 1$ we have from (11.5)

$$\Delta f^{[1]}(\delta) = a_2(\delta)\, l_2, \tag{12.3}$$

where a superscript $[m]$ denotes truncation of the sum in (11.5) at $n = m$. By the inequalities $l_2 \geqslant 0$ and $l_3 = \frac{1}{3} - \frac{2}{3}l_2$ (see (8.5)), there are just two vertices, $\boldsymbol{v}_0$ and $\boldsymbol{v}_1$, given by $l_2 = 0$ and $l_2 = \frac{1}{2}$, respectively. The first is clearly $\boldsymbol{v}_0 = \langle 3\rangle$, the (3, 3) antiphase state; the second likewise is $\boldsymbol{v}_1 = \langle 2\rangle$. Next note from (11.6) that $a_2(\delta)$ increases monotonically with δ (independently of the values of x and w). Hence the structure $\langle 3\rangle$ is realized for $\delta < \delta_1^{(1)}$, while $\langle 2\rangle$ is realized for $\delta > \delta_1^{(1)}$, where

$$a_2(\delta_1^{(1)}) = 0, \tag{12.4}$$

defines the first stage transition boundary $\delta_1^{(1)}$ (see (4.9) and (9.16)).

(ii) *Second order.* When $n = 2$ we are already in the $k = 0$ situation contemplated in proposition 1 of the previous section. To discuss the stability of the transition boundary $\delta = \delta_1^{(1)}$, we need thus consider only the additional structural variable l_{23}. In this case we obtain the

whole structural space $\mathscr{L}_2 = \{l_2, l_{23}\}$. For $\delta = \delta_1^{(1)}$ we have from (11.5) and the condition (12.4) simply

$$\Delta f^{[2]}(\delta_1^{(1)}) = a_{23}(\delta_1^{(1)})\, l_{23}. \tag{12.5}$$

Next observe from (12.1) that a_{23} is positive and hence conclude that for $\delta = \delta_1^{(1)}$ the realizable structure with maximal l_{23} will have a more favourable free energy than implied by either $\langle 2\rangle$ or $\langle 3\rangle$. By continuity this must also hold for some vicinity of $\delta_1^{(1)}$. To identify this appropriate structure we appeal to an almost obvious result, needed also in higher orders:

LEMMA 3. *The structural variable $l_{\mu^\dagger}$ with $\mu^\dagger = 2^k3$ $(k \geqslant 0)$ assumes its maximal value, namely $1/(2k+3)$, on the unique, realizable, periodic structure $\langle\mu^\dagger\rangle$ which is a vertex of $\mathscr{P}_n$ for all $n \geqslant k+1$. Furthermore, one has*

$$l_2(\langle\mu^\dagger\rangle) = k/(2k+3), \tag{12.6}$$

and for the standard structural variables, ν,

$$l_\nu(\langle\mu^\dagger\rangle) = \begin{cases} 1/(2k+3), & \text{for} \quad \nu = 2^j3, \quad j = 1, 2, \ldots, k, \\ 0, & \text{for all other} \quad \nu \neq 2. \end{cases} \tag{12.7}$$

Proof. First note that $\mu^\dagger$ is not subperiodic (or *self-matching*) in the sense of §8, or, phrased differently but equivalently, it does not have a structure that can be overlapped on itself, like, for example, $\mu = \mu_1\mu_2\mu_1$ in the sequence $\ldots\mu_1\mu_2\mu_1\mu_2\mu_1\ldots$. Thus any infinite structure with $l_{\mu^\dagger} > 0$ can be written $\ldots\mu_{j-1}\mu^\dagger\mu_j\mu^\dagger\mu_{j+1}\ldots = \Pi_j(\mu^\dagger\mu_j)$, where μ_j contains no $\mu^\dagger$ sequences. Clearly the density of $\mu^\dagger$ sequences, and hence $l_{\mu^\dagger}$, can be increased by deleting some μ_j and 'sliding' the remaining sequences along until one or more $\mu^\dagger$ can be inserted. Conversely, since $\mu^\dagger$ is not self-matching, one cannot increase the density by overlapping in any way. After successive deletions (up to periodic end effects for $L < \infty$) one obtains merely the structure $\ldots\mu^\dagger\mu^\dagger\mu^\dagger\ldots = \langle\mu^\dagger\rangle$, which is unique up to an axial translation. By inspection, $l_{\mu^\dagger}(\langle\mu^\dagger\rangle) = 1/(2k+3)$, which is thus the maximal value of $l_{\mu^\dagger}$. Finally, by choosing the objective function $\Phi(\boldsymbol{l}) = l_{\mu^\dagger}(\boldsymbol{l})$ on $\mathscr{L}_n$ with $n \geqslant k+1$, which is clearly maximized on $\boldsymbol{l} = \langle\mu^\dagger\rangle$ which satisfies all possible constraints, we prove $\langle\mu^\dagger\rangle$ is a vertex of $\mathscr{P}_n$. Alternatively, note that $\langle\mu^\dagger\rangle$ saturates the inequalities (10.9) since $l_\mu = 0$ whenever μ contains a subsequence 32^j3 with $0 < j < k$ or 2^j with $j > k$.

Finally note that (12.6) follows trivially by inspection of $\langle\mu^\dagger\rangle$ and the definition of l_2. The same is true for the first part of (12.7). To prove the second part, we once again classify the cores, $\tilde{\nu}$, of the ν by the number of 3-bands contained. If there is no 3-band, or $\tilde{\nu} = 2^j$, and $j \leqslant k$ applies, one merely recaptures the first part of (12.7); for $j > k$ the required result is obvious. If there is one 3-band, so that $\tilde{\nu} = 2^i32^j$, clearly only $0 \leqslant i, j \leqslant k$ need be considered. Under convention A one has $\nu = \nu_A = 2^{i+1}32^j3$, so that $l_\nu(\mu^\dagger) = 0$ unless $j = k$; but then ν is subperiodic unless $i = k$, which, in turn, also implies $l_\nu(\mu^\dagger) = 0$. In the last case, $i < k$, however, one must take $\nu = \nu_B = 32^i32^{k+1}$, which likewise confirms (12.7). With two 3-bands one clearly need consider only $\tilde{\nu} = 2^i32^k32^j$ with $i, j \leqslant k$; but the argument then goes through just as before, and likewise for three or more 3-bands.

Application of this lemma with $k = 1$ finally establishes that the new vertex at stage $n = 1$ is $\langle 23\rangle$, which is then stable for δ in the vicinity of $\delta_1^{(1)}$. More concretely, it is stable in the interval $\delta_1^{(2)} < \delta < \delta_2^{(2)}$, where the new boundaries may be defined (up to appropriate order) by

$$\Delta f_{\langle 3\rangle}(\delta_1^{(2)}) = \Delta f_{\langle 23\rangle}(\delta_1^{(2)}) \quad \text{and} \quad \Delta f_{\langle 23\rangle}(\delta_2^{(2)}) = \Delta f_{\langle 2\rangle}(\delta_2^{(2)}), \tag{12.8}$$

where for brevity we write

$$\Delta f_{\langle\mu\rangle}(\delta) = \Delta f(\{l_\nu\langle\mu\rangle\};\, \delta), \tag{12.9}$$

but where to the required order, $n = 2$, one can replace Δf by $\Delta f^{[2]}$ in (12.8). From (12.6) and (12.7) we thus find the determining expressions

$$a_2(\delta_1^{(2)}) + a_{23}(\delta_1^{(2)}) = 0, \quad \text{and} \quad \tfrac{3}{2}a_2(\delta_2^{(2)}) = a_{23}(\delta_2^{(2)}). \tag{12.10}$$

(iii) *Third order*. For $n = 3$ consider, first, the boundary $\langle 3\rangle$–$\langle 23\rangle$, i.e. δ in the vicinity of $\delta_1^{(2)}$. According to proposition 2 with $k = 1$ it is necessary in leading order to introduce only the new structural variable l_{233} and consider those corresponding $\boldsymbol{u}^{(3)}$, which on projection on to $\mathscr{P}_2$ lie on the edge

$$\boldsymbol{e}_{1-}(\theta) = \theta\langle 23\rangle + (1-\theta)\langle 3\rangle, \tag{12.11}$$

where one finds, using (12.6) and (12.7),

$$l_2(\theta) = l_{23}(\theta) = \tfrac{1}{5}\theta. \tag{12.12}$$

From (11.5) and (12.10) one then gets

$$\begin{aligned}\Delta f^{[3]}(\delta_1^{(2)}) &= \tfrac{1}{5}\theta[a_2(\delta_1^{(2)}) + a_{23}(\delta_1^{(2)})] + a_{233}(\delta_1^{(2)})\, l_{233} + O(w^{5q_\perp} l_{2333}) \\ &= a_{233}(\delta_1^{(2)})\, l_{233} + O(w^{5q_\perp} l_{2333}).\end{aligned} \tag{12.13}$$

Next observe from (12.2), with $k = 1$, that a_{233} is always negative. Hence the maximal value of $\Delta f^{[3]}$ is given by $l_{233} = 0$. But this simply means that the transition from $\langle 3\rangle$ to $\langle 23\rangle$ at $\delta = \delta_1^{(2)}$ is stable: no new maximal vertex appears. Thus there is a genuine phase transition from $\langle 3\rangle$ to $\langle 23\rangle$ at δ_1 in *all orders*. An evaluation of the interfacial free energy of the coexisting phases at δ_1 (see the next section) gives a positive value, so the transition is of first order. Note the exact transition point $\delta_1 \equiv \delta_1^{(\infty)}$ is given by solving the first member of (12.8) exactly, i.e. to all orders.

Secondly, consider the boundary $\langle 23\rangle$–$\langle 2\rangle$, i.e. the vicinity of $\delta_2^{(2)}$. This is completely analogous to the second-order situation where we appealed to proposition 1, except that now $k = 1$. The only new structural variable needed is thus l_{223} and, by (12.1), $a_{223}(\delta)$ is positive. Any feasible $\boldsymbol{u}^{(3)}$ must also project on to the edge

$$\boldsymbol{e}_{2,\infty}(\theta) = \theta\langle 23\rangle + (1-\theta)\langle 2\rangle, \tag{12.14}$$

where from (12.7) and (12.8) one finds

$$l_2(\theta) = \tfrac{1}{2} - \tfrac{3}{10}\theta, \quad l_{23}(\theta) = \tfrac{1}{5}\theta, \tag{12.15}$$

so that on using (12.10) one obtains

$$\Delta f^{[3]}(\delta_2^{(2)}) = \tfrac{1}{2}a_2(\delta_2^{(2)}) + a_{223}(\delta_2^{(2)})\, l_{233}. \tag{12.16}$$

But, since the first term is merely a constant, the maximum is attained on a new vertex $\langle 2^{k+1}3\rangle = \langle 223\rangle$ and the boundary line $\langle 23\rangle$–$\langle 2\rangle$ is unstable. New third-order transition boundaries are defined by

$$\Delta f_{\langle 23\rangle}(\delta_2^{(3)}) = \Delta f_{\langle 223\rangle}(\delta_2^{(3)}) \quad \text{and} \quad \Delta f_{\langle 223\rangle}(\delta_3^{(3)}) = \Delta f_{\langle 2\rangle}(\delta_3^{(3)}). \tag{12.17}$$

This completes the analysis to order $n = 3$.

(iv) *General order*. Evidently one can proceed by induction. In order $n = k+1$ first define the transition boundaries generally by

$$\Delta f^{[k+1]}_{\langle 2^{k-1}3\rangle}(\delta_k^{(k+1)}) = \Delta f^{[k+1]}_{\langle 2^k 3\rangle}(\delta_k^{(k+1)}), \tag{12.18}$$

$$\Delta f^{[k+1]}_{\langle 2^k 3\rangle}(\delta_{k+1}^{(k+1)}) = \Delta f^{[k+1]}_{\langle 2\rangle}(\delta_{k+1}^{(k+1)}). \tag{12.19}$$

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On using (12.6) and (12.7) to evaluate $\Delta f_{\langle 2^k 3\rangle}$, these yield the explicit equations

$$\tfrac{3}{2}a_2(\delta_k^{(k+1)}) + (k+\tfrac{1}{2})\,a_{2^k3}(\delta_k^{(k+1)}) = \sum_{j=1}^{k-1} a_{2^j3}(\delta_k^{(k+1)}), \quad k = 1, 2, 3, \ldots, \tag{12.20}$$

$$\tfrac{3}{2}a_2(\delta_{k+1}^{(k+1)}) = \sum_{j=1}^{k} a_{2^j3}(\delta_{k+1}^{(k+1)}), \quad k = 0, 1, 2, \ldots. \tag{12.21}$$

Evidently, we also need to evaluate the free energy contributions from the edges in order $n = k+2$, namely

$$e_{k-}(\theta) = \theta\langle 2^k 3\rangle + (1-\theta)\langle 2^{k-1}3\rangle \quad \text{at} \quad \delta = \delta_k^{(k+1)}, \tag{12.22}$$

$$e_{k+1,\infty}(\theta) = \theta\langle 2^k 3\rangle + (1-\theta)\langle 2\rangle \quad \text{at} \quad \delta = \delta_{k+1}^{(k+1)}. \tag{12.23}$$

By the linearity of the structural expansion for Δf and the defining equations (12.18) and (12.19), we find that on the edges one has, for all $0 \leqslant \theta \leqslant 1$,

$$\Delta f^{[k+1]}(\delta_k^{(k+1)}) \equiv \Delta f^{[k+1]}_{\langle 2^{k-1}3\rangle}(\delta_k^{(k+1)}) = \Delta f^{[k+1]}_{\langle 2^l 3\rangle}(\delta_k^{(k+1)}), \tag{12.24}$$

$$\Delta f^{[k+1]}(\delta_{k+1}^{(k+1)}) \equiv \Delta f^{[k+1]}_{\langle 2^k 3\rangle}(\delta_{k+1}^{(k+1)}) = \Delta f^{[k+1]}_{\langle 2\rangle}(\delta_{k+1}^{(k+1)}), \tag{12.25}$$

where, as regards the structural variables, the right-hand sides are constants. Higher-order contributions arise only from $l_{2^{k+1}3}$ at $\delta = \delta_{k+1}^{(k+1)}$ and, in leading order, from $l_{2^k32^{k-1}3}$ at $\delta = \delta_k^{(k+1)}$.

Finally, the positivity of $a_{2^k3}(\delta)$ ensures that *each structure* $\langle 2^{j-1}3\rangle$ *with* $j = 1, 2, 3, \ldots$, *appears sequentially as a new maximal vertex*. Conversely, the negativity of $a_{2^k32^{k-1}3}(\delta)$ ensures the *stability* of the boundaries $\delta_k^{(k+1)}$, which must then be identified as yielding true phase transitions from $\langle 2^{k-1}3\rangle$ to $\langle 2^k 3\rangle$ on the locus $\delta_k \equiv \delta_k^{(\infty)}$ (defined by letting $k \to \infty$ in the superscripts in (12.18)). In conclusion, then, we have established the existence at low temperatures with increasing κ (or δ) of the infinite sequence of phases $\langle\infty\rangle$, $\langle 3\rangle$, $\langle 23\rangle$, $\langle 223\rangle$, ..., $\langle 2^{j-1}3\rangle$, ..., $\langle 2\rangle$. No other phase can be present at sufficiently low temperatures and a phase occurs for every j.

13. Phase boundaries and surface tensions

Using the results established in the previous section for the sequence of phases and their boundaries, we will now establish recursion relations between successive boundaries which will enable us to estimate the 'width', in the (T, κ) plane, of the $\langle 2^k 3\rangle$ phase for large k. In addition, we will calculate explicitly in leading order the surface tension, $\Sigma_k(T)$, between successive phases $\langle 2^{k-1}3\rangle$ and $\langle 2^k 3\rangle$, i.e. on the phase boundary $\delta = \delta_k(T)$; the positivity of this surface tension will confirm the first-order character of the phase boundaries. (One might for this latter purpose, however, equally look at discontinuities in the entropy or energy, or in, say, $\partial f/\partial\kappa$ which measures the axial second neighbour spin–spin correlation function.) We may recall that $\delta_0(T)$ and $\Sigma_0(T)$ represent the boundary and corresponding surface tension between the ferro- or $\langle\infty\rangle$-phase and the $\langle 3\rangle$ or (3, 3) antiphase state. These are given explicitly in leading orders in (5.3) and (5.5) (see also figures 1 and 2). The (2, 2) antiphase state $\langle 2\rangle$ may be identified formally with $\langle 2^\infty 3\rangle$ and its boundary is $\delta_\infty(T)$.

From the structural expansion, (11.1)–(11.5), and the values for l_ν following from lemma 3 [(12.6) and (12.7)], the partial free energy in the phase $\langle 2^k 3\rangle$ is

$$\Delta f_k(\delta) \equiv \Delta f_{\langle 2^k 3\rangle} = \frac{k}{2k+3}\,a_2(\delta) + \frac{1}{2k+3}\sum_{j=1}^{k} a_{2^j3}(\delta), \tag{13.1}$$

and, clearly,
$$\Delta f_{\langle 2\rangle} \equiv \Delta f_{\infty}(\delta) = \tfrac{1}{2}a_2(\delta), \tag{13.2}$$
where, as before, the arguments x and w are understood and remain fixed at fixed T.

It is convenient to define first the unstable or pseudo-phase boundaries, $\delta_k^+(T)$, between $\langle 2^{k-1}3\rangle$ and $\langle 2\rangle$ (corresponding with $\delta_k^{(k)}$ of the previous section) formally via
$$\Delta f_{k-1}(\delta_k^+) = \Delta f_{\infty}(\delta_k^+). \tag{13.3}$$
By (13.1) and (13.2) this yields (see also (12.20))
$$3a_2(\delta_k^+) - 2\sum_{j=1}^{k-1} a_{2^j3}(\delta_k^+) = 0, \tag{13.4}$$
and, on replacing k by $k+1$,
$$3a_2(\delta_{k+1}^+) - 2\sum_{j=1}^{k-1} a_{2^j3}(\delta_{k+1}^+) = 2a_{2^k3}(\delta_{k+1}^+), \tag{13.5}$$
where we see from (11.2) and (12.1) that the right-hand side is of order $w^{(k+1)q_\perp}$. Now note that from (11.6) and (12.1) one has
$$(\partial a_2/\partial\delta) = \tfrac{4}{3}K_1 + O(w^{q_\perp}), \tag{13.6}$$
$$(\partial a_{2^j3}/\partial\delta) = O(w^{(j+1)q_\perp}), \quad \text{for} \quad j = 1, 2, \ldots, \tag{13.7}$$
where one should also note that δ is of order $w^{q_\perp}$. Then expanding (13.5) to first order in $\delta_{k+1}^+ - \delta_k^+$ and using (13.4) yields the basic recursion relation
$$K_1\,\delta_{k+1}^+ = K_1\,\delta_k^+ + \tfrac{1}{2}a_{2^k3}(0)\,[1 + O(w^{q_\perp})], \tag{13.8}$$
valid for $k \geqslant 1$, where one is allowed to put $\delta = 0$ in the coefficient a_{2^k3} because $\delta_k^+ = O(w^{q_\perp})$. Using (12.1) for a_{2^k3} gives a more explicit result. Note that $\delta_1^+ \equiv \delta_1^{(1)}$ is given to leading order in (4.11).

We have already seen that the boundaries represented by $\delta_k^+(T)$ are unstable against the formation of new, interpolating phases, but it is instructive to calculate formally the surface tension, $\Sigma_k^+(T)$, between domains of $\langle 2^{k-1}3\rangle$ phase and $\langle 2\rangle$ phase on such a boundary, to reconfirm the instability. Thus consider an overall lattice structure $(2^k3)^j 2^i$ connected periodically with i and j both of order L, the number of layers. Such a structure contains precisely two $\langle 2^k3\rangle{:}\langle 2\rangle$ interfaces. Furthermore, its reduced free energy is found to be
$$\Delta f_{\langle 2^k3\rangle:\langle\infty\rangle} = \frac{kj+i}{L}\,a_2(\delta) + \frac{j}{L}\sum_{h=1}^{k} a_{2^h3}(\delta) + \frac{1}{L}\sum_{h=k+1}^{i+k} a_{2^h3}(\delta) + O(w^{(2k+3)q_\perp}). \tag{13.9}$$
The first term and the two sums in this expression follow easily from the general structural expansion (11.1)–(11.4). To check the correction term notice that we require uncounted standard sequences of length $k+1$ or greater which must be of class A or class B (see the conventions of §8). Of the first class the leading non-vanishing sequences are clearly of the form $\mu \equiv \nu_{\mathrm{A}} = 2^l32^k3$. However, if $l \leqslant k$ such a μ would be subperiodic, and the required nonvanishing standard structures are $\mu \equiv \nu_{\mathrm{B}} = 32^{l-1}32^{k+1}$; but then l_μ vanishes, since $l-1 < k$. For $l > k$ the corresponding l_μ do not vanish, but such variables occur only in orders $n = l+k+2 \geqslant 2k+3$. Similarly, all class B sequences of form $\mu \equiv \nu_{\mathrm{B}} = 32^k32^l$ can be standard sequences only for $l > k$, but then the non-vanishing l_μ again occur only at orders $n \geqslant 2k+3$.

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Now evaluate (13.9) on the locus $\delta = \delta^+_{k+1}$ defined by (13.5): with $\theta = 2i/L$ and noting that $L = 2i + (2k+3)j$, the result can be rewritten

$$\Delta f_{k:\infty} \equiv \Delta f_{\langle 2^k 3\rangle:\langle\infty\rangle} = \theta a_2(\delta^+_{k+1}) + (1-\theta)\left[\frac{2k}{2k+3}\, a_2(\delta^+_{k+1}) + \frac{1}{2k+3}\sum_{h=1}^{k} a_{2^h 3}(\delta^+_{k+1})\right] + L^{-1}\sum_{h=k+1} a_{2^h 3}(\delta^+_{k+1}) + O(w^{(2k+3)q_\perp}). \tag{13.10}$$

But since the surface tension is defined as an excess free energy we have

$$-2\Sigma^+_{k+1}/k_B T \equiv L\{\Delta f_{k:\infty}(\delta^+_{k+1}) - [\theta \Delta f_\infty(\delta^+_{k+1}) + (1-\theta)\,\Delta f_k(\delta^+_{k+1})]\} = \sum_{h=k+1} a_{2^h 3}(\delta^+_{k+1}) + O(w^{(2k+3)q_\perp}), \tag{13.11}$$

the factor 2 on the left arising since there are *two* interfaces in the overall structure. To leading order it suffices to appeal to the basic result (12.1) to obtain

$$\Sigma^+_{k+1}/k_B T = -\tfrac{1}{2}(k+3)\,(1+x)\,(1-x)^{k+3} w^{(k+2)q_\perp}[1 + O(w^{q_\perp})]. \tag{13.12}$$

For $x < 1$ this expression is negative thence providing an alternative demonstration of the instability of the boundary $\langle 2^k 3\rangle$–$\langle 2\rangle$.

Now the true phase transition boundaries, $\delta = \delta_k(T)$, are defined by equating Δf_{k-1} and Δf_k: after some manipulation this yields

$$3a_2(\delta_k) - 2\sum_{j=1}^{k-1} a_{2^j 3}(\delta_k) + (2k+1)\, a_{2^k 3}(\delta_k) = 0, \tag{13.13}$$

for $k \geqslant 1$ (see also (12.21)). A comparison with (13.4) indicates that an expansion in powers of $\delta_k - \delta^+_k$ is appropriate. In first order this yields the required relation

$$K_1 \delta_k = K_1 \delta^+_k - \tfrac{1}{2}(k+\tfrac{1}{2})\, a_{2^k 3}(0)\,[1 + O(w^{q_\perp})]. \tag{13.14}$$

By replacing k by $k+1$ and using the recursion relation for δ^+_k, a direct relation between δ_{k+1} and δ_k can be obtained. We postpone the details, however, until the next section.

Finally, let us compute the surface tension on the phase boundary $\delta_k(T)$. To this end consider the overall periodic lattice structure $(2^{k-1}3)^i(2^k 3)^j$ which has two interfaces in a total number of layers $L = (2k+1)i + (2k+3)j$ and contains a volume fraction $\theta = (2k+1)i/L$ of the phase $\langle 2^{k-1}3\rangle$. From the structural expansion the reduced free energy is found to satisfy

$$L\Delta f_{\langle 2^{k-1}3\rangle:\langle 2^k 3\rangle} = i\left[(k-1)\,a_2 + \sum_{h=1}^{k-i} a_{2^h 3}\right] + j\left[k a_2 + \sum_{h=1}^{k} a_{2^h 3}\right] + a_{2^k 3 2^{k-1} 3} + O(w^{(3k+1)q_\perp}). \tag{13.15}$$

The first two terms follow easily and exhaust all standard sequences, ν, with no 3-bands in their cores, $\tilde{\nu}$. Cores with one 3-band yield class A sequences $\mu = 2^l 3 2^{l'} 3$, and an analysis along the now familiar lines employing the A and B conventions shows that only $l = k$ and $l' = k-1$ can be nonvanishing. Similarly, by subclassifying all cores with two 3-bands and using the conventions, one establishes the order of the correction term. Comparison with (13.1) and defining the surface tension $\Sigma_k(T)$ in terms of the excess free energy in precise analogy to the first part of (13.11), then yields the conclusion

$$\Sigma_k(T)/k_B T = -\tfrac{1}{2} a_{2^k 3 2^{k-1} 3}(\delta_k)\,[1 + O(w^{kq_\perp})]. \tag{13.16}$$

On using the basic expression (12.2) this gives, more explicitly,

$$\Sigma_k(T)/k_B T = \tfrac{1}{2}x(1-x)^{2k+2}w^{(2k+1)q_\perp}[1+O(w^{q_\perp})]. \tag{13.17}$$

Evidently this is positive (for $x < 1$) in agreement with the anticipated stable and first-order character of the phase transition boundary $\delta = \delta_k(T)$ between phases $\langle 2^{k-1}3\rangle$ and $\langle 2^k 3\rangle$.

14. Wavevector variation and phase widths

To obtain an expression, more accurate than (4.11), for $\delta_1^+ \equiv \delta_1^{(1)}(T)$, the initial locus or pseudo-phase boundary defined by the vanishing of $a_2(\delta)$, one may use the explicit third-order analysis of §9 and solve for δ_1^+ in powers of w. This yields

$$\begin{aligned} K_1\delta_1^+ = {} & (1-x)^2(1+\tfrac{1}{2}x)\,w^{q_\perp} + \tfrac{1}{2}q_\perp(1-x^2)^2(1+\tfrac{1}{2}x^2)\,w^{2q_\perp-2} \\ & + \tfrac{1}{2}w^{2q_\perp}[-(q+\tfrac{5}{2}) + 12x + \tfrac{3}{2}(q-7)x^2 - 8x^3 + \tfrac{21}{2}x^4 - \tfrac{1}{2}(q+3)] \\ & + p_3 w^{3q_\perp-6}(1-x^3)(1+\tfrac{1}{2}x^3) + c_2 w^{3q_\perp-4}(1-x^3)^2(1+\tfrac{1}{2}x^3) + O(w^{3q_\perp-2}), \end{aligned} \tag{14.1}$$

where $q = q_\perp + 2$ and p_3 and c_2 are defined in table 3.

We may also refine the recursion relations (13.8) and (13.14) by carrying out an expansion of $a_2(\delta)$ to leading order about $\delta = \delta_1^+$ so as to capture the first correction term in (13.6). One thence obtains

$$K_1\delta_{k+1}^+ = K_1\delta_k^+ + \tfrac{1}{2}a_{2k3}(\delta_1)\,[1+6w^{q_\perp}x(1-\tfrac{1}{3}x^2) + O(w^{2q_\perp-2})], \tag{14.2}$$

$$K_1\delta_k = K_1\delta_k^+ - \tfrac{1}{2}(k+\tfrac{1}{2})\,a_{2k3}(\delta_1)\,[1+6w^{q_\perp}x(1-\tfrac{1}{3}x^2) + O(w^{2q_\perp-2})]. \tag{14.3}$$

If we use (12.1) and write

$$y = w^{q_\perp}\{1 - x\exp[-4w^{q_\perp}(1-x)^2(1+\tfrac{1}{2}x) + O(w^{2q_\perp-2})]\}, \tag{14.4}$$

which becomes small as $w = \exp(-2J_0/k_B T) \to 0$, these recursion relations can be rewritten as

$$\delta_k = \delta_k^+ - c(k+\tfrac{1}{2})(k+2)\,y^{k+1}, \tag{14.5}$$

$$\delta_{k+1}^+ = \delta_k^+ + c(k+2)\,y^{k+1}, \tag{14.6}$$

for $k = 1, 2, \ldots$, where

$$c = \tfrac{1}{2}K_1^{-1}(1-x^2)\,[1+6w^{q_\perp}x(1-\tfrac{1}{3}x^2) + O(w^{2q_\perp-2})]. \tag{14.7}$$

The *width* or *extent*, $\Delta\delta_k$, of the phase $\langle 2^k 3\rangle$ at constant T is naturally defined by $\delta_{k+1} - \delta_k$ which follows immediately from (14.5) and (14.6) as

$$\Delta\delta_k \equiv \delta_{k+1} - \delta_k = c(k+\tfrac{3}{2})(k+2)\,[1 - y(k+3)/(k+2)]\,y^{k+1}. \tag{14.8}$$

For large k this shows that the *widths decrease exponentially rapidly* varying, for small x, as $k^2\exp(-2kJ_0/k_B T)$. By using (14.5) with $k = 1$ to determine the true $\langle 3\rangle\langle 23\rangle$ boundary, $\delta_1(T)$, the result (4.8) also provides a direct recursion relation for the phase boundaries $\delta_k(T)$ without reference to the pseudo-phase boundaries $\delta_k^+(T)$.

To study the approach to the limiting locus, $\delta_\infty(T)$, which bounds the $\langle 2\rangle$ phase, we may approximate $(k+3)/(k+2)$ by 1 for $k \to \infty$ and treat (14.8) approximately as a differential equation in k. On neglecting terms of order $1/\ln y^{-1} = O(k_B T/J_0)$ one can integrate to obtain

$$\delta_\infty - \delta_k \approx c(1-y)\,|\ln y|^{-1}(k^2 + \tfrac{7}{2}k + 3)\,y^{k+1}. \tag{14.9}$$

It is of interest to relate the phase transitions with the change of wavevector. The mean wavevector $\bar{q} = |\bar{\boldsymbol{q}}|$ of the phase $\langle 2^k 3\rangle$ for $k = 0, 1, 2, \ldots$ is just

$$q_k = q_{\langle 2\rangle}[1-(2k+3)^{-1}], \tag{14.10}$$

where $q_{\langle 2\rangle} = q_\infty = \pi/2a$ is the wavevector of the $\langle 2\rangle$ phase. To study the variation of the wavevector $\bar{q}(T, \kappa)$ it is convenient to introduce a normalizing factor

$$\Delta_0(T) = (k_B T/J_1)\, e^{-2q_\perp J_0/k_B T}[1+X(T)], \tag{14.11}$$

with

$$1+X(T) = (1-x)(1-x^2)[1+6xy(1-\tfrac{1}{3}x^2)/(1-x)], \tag{14.12}$$

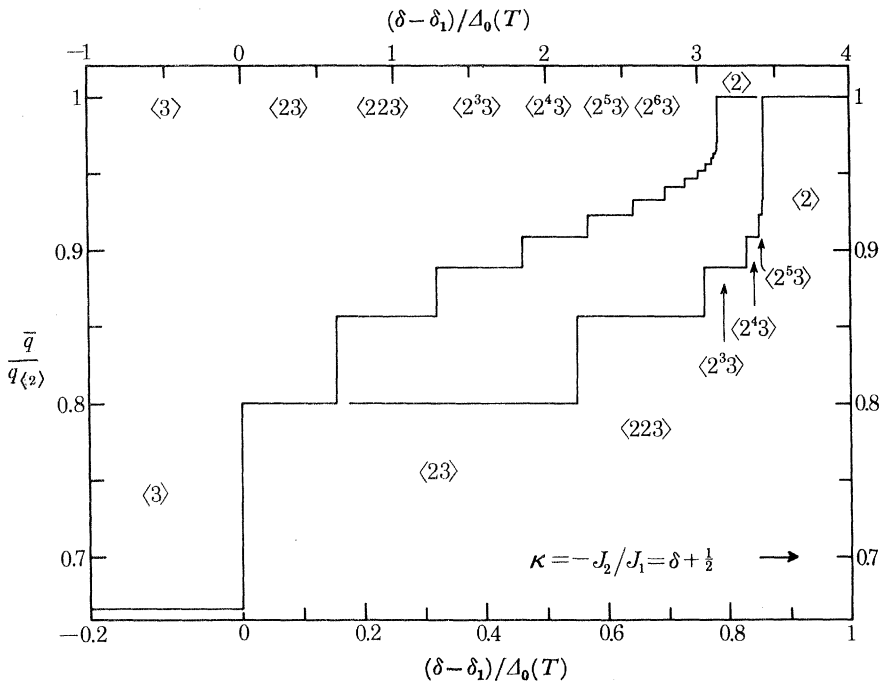

FIGURE 6. Variation of the mean wavevector $\bar{q}(T, \kappa)$ with $\kappa = \frac{1}{2}+\delta$ at fixed, low temperature showing the sequence of commensurate equilibrium phases. The scale $\Delta_0(T) \sim \exp(-2q_\perp J_0/k_B T)$ is defined precisely in (14.11), while $\delta_1(T) \approx \delta_1^+(T)$ (see (14.1)) represents the $\langle 3\rangle\langle 23\rangle$ boundary. The upper plot and scale refer to $y = 0.5$, while the lower plot and scale are for $y = 0.2$, where $y \approx \exp(-2q_\perp J_0/k_B T)$ is defined in (14.4).

where, as before, $x = \exp(-2J_1/k_B T)$. Then the recursion relation (14.8) may be written

$$\delta_{k+1} = \delta_k + \tfrac{1}{2}\Delta_0(T)(k+\tfrac{3}{2})[k+2-y(k+3)]y^k. \tag{14.13}$$

This has been used with (14.10) to generate the plots of $\bar{q}(T, \kappa)$ for fixed T shown in figure 6. (See also figure 2 of Fisher & Selke (1980).)

Evidently, for low temperatures, $\bar{q}$ varies in a staircase fashion but with an accumulation of infinitely many, infinitely small steps at the boundary, $\delta_\infty(T)$, of the $\langle 2\rangle$ phase – a 'devil's top step'. As is clear on extending figure 5 to all k, the situation is similar if the $\langle 2\rangle$ phase is heated at constant $\kappa > \frac{1}{2}$ (or $\delta > 0$). Initially the wavevector remains locked at $\bar{q} = q_\infty \equiv q_{\langle 2\rangle} = \pi/2a$, corresponding to the periodic sequence of two up – two down spin layers, although the magnetization modulation, $M_0(T)$, of the magnetization modulation deviates below saturation

as T increases. However, on reaching a limiting temperature, $T_{\mathrm{m}}(\kappa)$, defined by $\delta_\infty(T_{\mathrm{m}}) = \kappa - \frac{1}{2}$, the $\langle 2\rangle$ phase 'melts' abruptly, although quasicontinuously, by nucleating a set of widely spaced but *equally* spaced bands of three up and three down spin layers (Fisher & Selke 1980). As T increases through T_{m}, the spacing between the 3-bands decreases rapidly via a series of discrete and increasingly strong first-order transitions. This corresponds to a 'soliton-like' mechanism (Bishop & Schneider 1978; Villain 1980) for melting and varying $\bar{q}$, although the successive equilibrium phases remain commensurate and locked to the lattice. The expression (14.8) can be interpreted as implying a repulsive interaction between adjacent 'solitons' or 3-bands which decreases exponentially with distance.

The limiting form of the variation of $\bar{q}(T, \kappa)$ for large k may be found by treating k as a continuous variable and inverting (14.9) to obtain k, and thence q_k, as a function of

$$\Delta = \delta_\infty - \delta_k. \tag{14.14}$$

This leads to

$$1 - \frac{\bar{q}}{q_{\langle 2\rangle}} \approx \frac{B(T)}{\ln \Delta^{-1} + 2\ln(C \ln \Delta^{-1})[1 + (2/\ln \Delta^{-1})] + B/\ln \Delta^{-1}}, \tag{14.15}$$

where

$$B(T) = \tfrac{1}{2} \ln y^{-1} \approx q_\perp J_0/k_{\mathrm{B}}\, T + x \exp\left[-4w^{q_\perp}(1-x)^2(1+\tfrac{1}{2}x)\right], \tag{14.16}$$

$$C(T) = \frac{(1+x)^{\frac{1}{2}}(1-x)^{\frac{1}{4}}}{4q_\perp^{\frac{3}{2}} K_1^{\frac{1}{2}} K_0^{\frac{3}{2}} w^{\frac{1}{4}q_\perp}}\left[1 + O(w^{q_\perp})\right]. \tag{14.17}$$

For large k, near the $\langle 2\rangle$ phase boundary, the wavevector thus varies quasicontinuously according to

$$q_{\langle 2\rangle}(T) - \bar{q}(T, \kappa) \sim 1/\ln\left[\delta_\infty(T) - \delta\right]^{-1} \tag{14.18}$$

(Fisher & Selke 1980). This form can again be interpreted as reflecting an exponentially decreasing repulsion between solitons.

This completes our analysis of the low temperature behaviour of the ANNNI models for dimensionalities $d > 2$. In the vicinity of the multiphase point at $(T = 0, \kappa = \frac{1}{2})$ we believe our results reveal the full phase diagram. The situation at intermediate temperatures, however, remains open on the basis of the present arguments: certainly the presence of a truly incommensurate phase, with $\bar{q}(T, \kappa)$ varying continuously with T and κ has not been ruled out. It is also possible that additional, discrete interpolating phases, such as $\langle 34\rangle$, or $\langle 233\rangle$, or $\langle 23223\rangle$, etc., appear as particular *nonzero* temperatures are reached, although our full third-order calculations suggest that such temperatures cannot be very low.

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Appendix: Calculation of structural coefficients to general order

By (11.1)–(11.5) the reduced free energy can be written

$$f(\{l_\mu\}) = a_0 + \sum_\nu a_\nu l_\nu = a_0 + \sum_\nu l_\nu b_\nu w^{q_\perp n_0(\nu)}, \tag{A 1}$$

where the sum runs over all standard sequences ν of span $n_0(\nu)$ (and band length $m(\nu)$). As demonstrated in §12, it suffices to establish the sequence of low-temperature phases in the ANNNI model to know the two special results

$$a_{\nu_k} = w^{(k+1)q_\perp}(k+2)(1-x^2)(1-x^{1+2\delta})^{k+1}[1+O(w^{q_\perp-2})], \tag{A 2}$$

$$a_{\nu_{kk}} = -w^{(2k+1)q_\perp}x^{1-2\delta}(1-x^{1+2\delta})^{2k+2}[1+O(w^{q_\perp-2})], \tag{A 3}$$

for all $k \geqslant 1$ where relevant structural sequences are

$$\nu_k \equiv 2^k3 \quad \text{and} \quad \nu_{kk} \equiv 2^k32^{k-1}3. \tag{A 4}$$

In this Appendix we outline the derivation of these results. We remark initially, however, that the sequence of phases and all the qualitative results established in §§12–14 rest only on the leading terms in x in (A 2) and (A 3) since, if $T \to 0$ at fixed J_0, J_1 and κ, both w *and* x approach zero. Many of the complications in the calculations presented below stem from the desire to obtain the full x-dependence of the terms of leading order in w.

Table 5. Low energy connected axial configurations

The power of x in the corresponding Boltzmann weight is denoted $\beta(\delta)$ (see (9.10)). Since the inversion (or reflexion) of a configuration with respect to the anisotropy axis leaves the energy invariant, such inversions are to be understood if not specifically listed.

m \ β	0	4δ	$1-2\delta$	$1+2\delta$
1	σ	—	—	τ
2	$\sigma\cdot\tau$ $\tau\cdot\sigma$	τ, τ	—	ρ, σ σ, ρ $\sigma\cdot\sigma$ $\tau\cdot\tau$
3	$\sigma\cdot\tau\cdot\tau$ $\tau\cdot\tau\cdot\sigma$ $\sigma, \rho\cdot\sigma$ $\sigma\cdot\rho, \sigma$	$\tau, \tau\cdot\tau$ $\tau\cdot\tau, \tau$ σ, ρ, σ	$\sigma\cdot\rho\cdot\sigma$	$\rho, \sigma\cdot\tau$ $\sigma, \rho\cdot\tau$ $\sigma/\tau, \tau$ $\sigma\cdot\sigma\cdot\tau$ $\tau\cdot\tau\cdot\tau$
$\geqslant 4$	$\sigma(\cdot\tau)^j$ $(\tau\cdot)^j\sigma$ $(j \geqslant 0)$ no others	$\tau, \tau(\cdot\tau)^j$ $(\tau\cdot)^i\tau, \tau(\cdot\tau)^j$ $(\tau\cdot)^i\sigma, \rho, \sigma(\cdot\sigma)^j$ $(i,j \geqslant 0)$, etc.	$\sigma\cdot(\tau\cdot)^i\rho(\cdot\tau)^j\cdot\sigma$ $(i,j \geqslant 0)$ no others spaced	$\tau(\cdot\tau)^j$ $(j \geqslant 0)$ etc.

The understanding of the arguments leading to (A 2) and (A 3) should be significantly aided by working through some of the analysis sketched in §9, where the general low temperature expansion is presented explicitly to third order. In particular, reference will be made to the nature of table 1 in second order and to its analogues in third and higher orders. Indeed, without working in detail through the low orders, it would be difficult to see the route to the appropriate calculations to all orders. In fact, (A 2) and (A 3) were initially examined in fourth and fifth orders (and may be checked in full in third order from the data given in table 3).

The first step in the derivation is to note, by using the result (8.13), that the spans of the relevant sequences, ν_k and ν_{kk}, are $k+1$ and $2k+1$, respectively, since there is only one 3-band

in the core $\tilde{\nu}_{kk} = 2^{k-1}32^{k-1}$ of ν_{kk}, and there are none in the core $\tilde{\nu}_k = 2^{k-1}$ of ν_k. The lowest-order contribution to the statistical weight of any spin configuration involving l_{ν_k} must thus involve $k+1$ overturned spins with no overturned neighbours in a layer; likewise $2k+1$ are required for ν_{kk}. These observations explain the powers of w appearing in (A 2) and (A 3); the correction factor arises from configurations with one (or more) in-layer neighbours.

It follows by the same arguments that one need consider *only axial configurations* of the three classes of overturned spins, ρ, σ, and τ (see (2.5)). The configurations of this sort having lowest energies, and hence contributing to the leading powers, β, in x, are listed in table 5. To read this table, note, from §9, that a comma separating two spin symbols denotes nearest axial neighbours in the same band, while a solidus refers to nearest neighbours in adjacent bands; a bold dot indicates second (or spaced) axial neighbours; a semicolon is used to mark off the connected components of separated (or disconnected) configurations.

Next observe, as evident from table 1 and consideration of, for example, (9.2), that a given standard structural variable l_ν arises not only from spin configurations spanning the standard sequence itself, but *also*, via the structural relations (8.2), from spin configurations spanning the *related sequences* which share a common core $\tilde{\nu}$. It follows that to determine a_{ν_k} one must study spin configurations spanning sequences of the types

$$(a)\ 2\tilde{\nu}_k 2, \quad (b)\ 2\tilde{\nu}_k 3, \quad 3\tilde{\nu}_k 2, \quad (c)\ 3\tilde{\nu}_k 3, \tag{A 5}$$

where, by inversion (or reflexion) symmetry with respect to the anisotropy axis, both members of type (*b*) contribute equally. Likewise, for $a_{\nu_{kk}}$ one needs the analogous three types since $2\tilde{\nu}_{kk}3 \equiv \nu$ is just the inverse of $3\tilde{\nu}_{kk}2 = 32^{k-1}32^k$ so that both again contribute equally. Now the structural relations (8.2) and (8.3) can be solved generally for the non-standard sequences associated with ν of class A (i.e. $\nu = 2\tilde{\nu}3$) as

$$\begin{aligned} (a)\ l_{2\tilde{\nu}2} &= l_{2\tilde{\nu}} - l_\nu, \\ (b)\ l_{3\tilde{\nu}2} &= l_{\tilde{\nu}} - l_{2\tilde{\nu}} - l_{\tilde{\nu}3} + l_\nu, \\ (c)\ l_{3\tilde{\nu}3} &= l_{\tilde{\nu}3} - l_\nu, \end{aligned} \tag{A 6}$$

in which all sequences appearing on the right, except ν, are of lower order (i.e. shorter in length, m) than ν. From this follows:

RULE 1. *Configurations spanning sequences of type* (*b*) *contribute positively to* a_{ν_k} *and* $a_{\nu_{kk}}$, *but those spanning sequences of types* (*a*) *and* (*c*) *contribute negatively.*

Another important feature can be seen from the first part of table 1, which lists the second-order separated configurations such as ρ; ρ (see also (9.3)). Specifically, contributions involving a sequence μ arise not only directly from connected contributions spanning μ but also indirectly from separated configurations, like $\omega = \omega_1; \omega_2; \ldots; \omega_p$. As evident from the arguments leading to (9.3), this occurs because, in reducing the count N_ω of a separated configuration ω of p components to a polynomial of degree p in N, the number of lattice sites, one must, in succession, subtract off the *overlaps* and *contacts* (at first neighbour and second axial neighbours) which can be generated by the components $\omega_1, \omega_2, \ldots$ as they are moved over the lattice without restriction (see also Domb 1960). Now to generate an *overlap* configuration spanning a sequence μ from a separated configuration ω, one must clearly have components of ω whose spans when totalled *exceed* the span of μ. The same conclusion holds for *contacts* cemented by in-layer bonds. In all such cases, however, the statistical weights will involve more powers of

$w^{q_\perp}$ than the span of μ. Hence such overlaps and in-layer contacts will contribute to a_{ν_k} and $a_{\nu_{kk}}$ only powers of $w^{q_\perp}$ greater than the leading terms. On the other hand, (non-overlapping) linear *axial contacts* such as, with $p = 3$, ω_1, ω_2/ω_3 or $\omega_1 \cdot \omega_2 \cdot \omega_3$, *will* contribute in leading order to the terms associated with a given μ.

It follows from this discussion that, in considering ν_k, ν_{kk}, and their related sequences, one must also consider non-overlapping but contacting axial spin configurations that can be decomposed into two, three, ..., p separated configurations. Such many-fold decompositions turn out, in fact, to play a crucial role and are directly responsible for the structure exhibited in (A 2) and (A 3). To make matters concrete some examples may be useful: consider, in fourth order, the type (c) sequence 32^23 which, as regards connected axial configurations, is spanned only by $\sigma\cdot\tau\cdot\tau\cdot\rho$, $\sigma\cdot\tau\cdot\tau/\sigma$, and $\sigma\cdot\tau/\tau\cdot\sigma$, all with energy corresponding to an exponent of x of $\beta = 2$. (The reader will find it helpful to draw diagrams of the band structures and spin configurations.) From the second and third configurations we derive the obvious twofold decompositions $\sigma\cdot\tau\cdot\tau$; σ and $\sigma\cdot\tau$; $\tau\cdot\sigma$ which, by table 5, have *lower* energy, corresponding only to $\beta = 0$. (Recall that the energies of separated configurations add over the components.) A threefold decomposition is $\sigma\cdot\tau$; τ; σ, but from table 5 this has higher energy with $\beta = 1 + 2\delta$. Likewise a fourfold decomposition is σ; τ; τ; σ with $\beta = 2 + 4\delta$. By proceeding systematically one can clearly make an exhaustive list of all possible decompositions and their energies.

The question now arises as to the magnitude and sign of the contribution of a given decomposition. It is suggested by the first part of table 1, and easily proved generally, that a twofold decomposition spanning a sequence μ always contributes with weight unity but with negative sign to the coefficient of l_μ. Conversely, because of the two successive stages of subtraction needed in reducing a count for a separated configuration of three components, one obtains a positive contribution of unit weight from a threefold decomposition. With a little thought it is not hard to develop an inductive argument for higher-order decompositions, in which the linearity of the decompositions plays a central role. Thence one establishes:

RULE 2. *Each p-fold decomposition of a configuration spanning a sequence μ contributes $-(-)^p 1$ to the coefficient of l_μ.*

Of course, in computing the contribution to the related standard variable, ν, one must also employ rule 1.

We are now in a position to undertake the calculation of a_{ν_k} and a $a_{\nu_{kk}}$. Consider, first, type (a) sequences related to ν_k, i.e. of the form $\mu = 2^{k+1}$. It is easy to see (again a diagram of the band structure is helpful) that the only connected spanning configurations are

$$(a)_k\,(\mathrm{i}) \quad \tau(\cdot\tau)^k \quad \text{with} \quad \beta = 1 + 2\delta, \quad g_0 = -2\bar{x},$$

$$(\mathrm{ii}) \quad \tau(\cdot\tau)^i/(\tau\cdot)^j\tau \quad (i+j = k-1), \quad \beta = 4 + 4\delta, \quad g_0 = -kx^2\bar{x}^2, \tag{A 7}$$

where for brevity we have written

$$\bar{x} = x^{1+2\delta}, \tag{A 8}$$

while g_0 denotes the total contribution of the corresponding connected configuration to a_{ν_k}: the minus signs follow from rule 1; the factor 2 for (i) arises because the initial τ spin can be one of two in a band; likewise in (ii) there are k positions for the cross-band contact (/) or, equivalently, there are k partitions satisfying $i + j = k - 1$ with $i, j \geqslant 0$.

Now the only decompositions of type (a)(i) are into components of the form $\tau(\cdot\tau)^j$ with $j \geqslant 0$; such a configuration of p components has $\beta = p(1+2\delta)$ (see table 5). Furthermore, because of the linearity of the configuration $\tau(\cdot\tau)^k$, it has precisely $\binom{k}{p-1}$ distinct p-fold decompositions where, clearly, $p \leqslant k+1$. On invoking rule 2, we thus see that the overall contribution made by type (a)(i) configurations together with their decompositions is just

$$(a)_k\,(\mathrm{i}) \quad \tau(\cdot\tau)^k\colon \quad g = -2\bar{x}(1-\bar{x})^k, \tag{A 9}$$

where the binomial theorem yields the compact expression.

Turning to the decompositions of type $(a)_k$(ii) configurations, we see they are of two sorts: either, by splitting $\tau(\cdot\tau)^i/(\tau\cdot)^j\tau$ at the cross-band contact $(/)$, just like those of type $(a)_k$(i); *or*, by breaking elsewhere, consisting of one component of type $(a)_k$(ii) with $i+j < k-1$, together with $(p-1)$ components of the previous type, $\tau(\cdot\tau)^i$, with $i \geqslant 0$. Carrying through the energetics and combinatorics as before then yields

$$(a)_k(\mathrm{ii}) \quad \tau(\cdot\tau)^i/(\tau\cdot)^j\tau, \quad (i+j = k-1, \quad i,j \geqslant 0)\colon$$
$$g = k\bar{x}^2(1-\bar{x})^{k-1} - kx^2\bar{x}^2(1-\bar{x})^{k-1}. \tag{A 10}$$

Similar arguments may now be applied to type (b) and (c) configurations related to ν_k and they yield

$$(b)_k(\mathrm{i}) \quad (\tau\cdot)^k\rho\colon \qquad g = 2x^2\bar{x}(1-\bar{x})^k, \tag{A 11}$$

$$(\mathrm{ii}) \quad \tau(\cdot\tau)^j/(\tau\cdot)^{k-j}\sigma \quad (0 \leqslant j \leqslant k)\colon \qquad g = 2kx^2\bar{x}(1-\bar{x})^{k-1} - 2k\bar{x}(1-\bar{x})^{k-1}, \tag{A 12}$$

$$(\mathrm{iii}) \quad (\tau\cdot)^k\sigma\colon \qquad g = 2(1-\bar{x})^k, \tag{A 13}$$

where, here and below, the corresponding inverted configurations have been counted but not displayed; and

$$(c)_k(\mathrm{i}) \quad \sigma(\cdot\tau)^{k-1}\cdot\rho\colon \qquad g = -2x^2(1-\bar{x})^k, \tag{A 14}$$

$$(\mathrm{ii}) \quad \sigma(\cdot\tau)^j/(\tau\cdot)^{k-1-j}\sigma \quad (0 \leqslant j \leqslant k-1)\colon \qquad g = -kx^2(1-\bar{x})^{k-1} + k(1-\bar{x})^{k-1}. \tag{A 15}$$

On summing the contributions g from (A 9)–(A 15) the result (A 2) for a_{ν_k} is obtained. One may notice that the leading contributions in x arise only from the connected configuration $(\tau\cdot)^k\sigma$ (of (A 13)) and from the twofold decompositions of $(c)_k$(ii) at the $(/)$ or cross-band contact. Enumeration of these low energy configurations would, as mentioned, suffice to establish the existence of the infinite sequence of phases $\langle 2^k3\rangle$ for $k = 1, 2, 3, \ldots$.

The consideration of the sequences ν_{kk} proceeds similarly. Matters are simpler because there is only one connected spanning configuration of each type, but the decompositions are now more complex, since *three* distinct types of separated configuration, e.g. $\tau(\cdot\tau)^i$, $(\tau\cdot)^i\rho(\cdot\tau)^j$, and $(\tau\cdot)^i\sigma$, can occur in a given p-fold decomposition. Nevertheless, after carefully going through the energetics and combinatorics the expressions reduce to the simple forms:

$$(a)_{kk} \quad (\tau\cdot)^k\rho(\cdot\tau)^k\colon \qquad g = -x^2\bar{x}(1-\bar{x})^{2k}, \tag{A 16}$$

$$(b)_{kk} \quad (\tau\cdot)^k\rho(\cdot\tau)^k\cdot\sigma\colon \qquad g = 2x^2(1-\bar{x})^{2k}, \tag{A 17}$$

$$(c)_{kk} \quad \sigma\cdot(\tau\cdot)^{k-1}\rho(\cdot\tau)^{k-1}\cdot\sigma\colon \qquad g = -x^{1-2\delta}(1-\bar{x})^{2k}. \tag{A 18}$$

When these three expressions are summed, the result (A 3) for $a_{\nu_{kk}}$ is finally established. Evidently, the leading term in x arises solely from the connected low energy configuration

$(c)_{kk}$. Thus to establish the stability of the $\langle 2^{k-1}3\rangle\langle 2^k 3\rangle$ boundaries, one only needs to identify this configuration and check that all other configurations and decompositions have higher energy: the combinatorics of the decompositions are not really required. However, the lack of any special peculiarities in the complete coefficient in x suggests that the character of the phase diagram in the multiphase region remains uniform as J_1/J_0 varies.

Lastly, we remark that the proof of rule 2 for general p is also not required for the leading results since, as commented after (A 15), only twofold decompositions need be enumerated explicitly once it is established that all the higher-order decompositions have higher energy.

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