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Perturbation expansions of the axial next-nearest-neighbour Ising and asymmetric four-state clock models

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Abstract. The axial next-nearest-neighbour Ising (ANNNI) and four-state asymmetric clock (4ASC) models are investigated by perturbing about points at which they reduce to simple nearest-neighbour Ising models. These limits are (a) for the ANNNI model—(i) small nearest-neighbour interaction, J_1, in the x direction and (ii) small next-nearest-neighbour interaction, J_2, in the x direction, and (b) for the 4ASC model small asymmetry, Δ. In the limit $J_1 \to 0$, the phase boundary is located to first order in J_1 and found to be Ising-like. In the limit $J_2 \to 0$, the behaviour to second order in J_2 is more complicated but is identical to that found to second order in Δ for the 4ASC model. These results are discussed in the light of other recent work.

1. Introduction

Systems exhibiting, or apparently exhibiting, incommensurate/commensurate transitions are currently of considerable interest; for a recent review see Villain (1980). In such a transition a commensurate phase with long-range order 'melts' to an incommensurate or 'floating' phase. The latter phase is characterised by a spatially modulated order parameter, the wavevector of the modulation being incommensurate with the underlying lattice. In two dimensions, an incommensurate phase, in addition, exhibits an algebraic decay of the order parameter correlation function and thus is expected to be similar to the low-temperature phase of the planar rotor model.

In an attempt to understand incommensurate/commensurate transitions in more detail, particularly in two dimensions, attention has focused on two simple models: the axial next-nearest-neighbour Ising or ANNNI model and the asymmetric clock models.

In two dimensions, the dimensionality of interest here, the ANNNI model is specified by the Hamiltonian

$$H = -\sum_{(i,j)} \left(J_1 s_{i,j} s_{i+1,j} - J_2 s_{i,j} s_{i+2,j} + J_0 s_{i,j} s_{i,j+1} \right) \tag{1.1}$$

where the sum is over all sites of a square lattice, each site being populated by an Ising spin $s_{i,j}(=\pm 1)$. All coupling constants, J_i, $i = 0, 1, 2$, are positive so that the nearest-neighbour interactions (J_0, J_1) are ferromagnetic while the axial next-nearest-neighbour interactions $(-J_2)$ are *antiferromagnetic*. It is this competition which leads to an incommensurately ordered phase for certain values of the couplings and temperature.

The three-dimensional version† of the model was originally proposed by Elliot (1961) to describe the modulated phase observed in some rare earths. The revival of interest stems from the work of Bak and von Boehm (1979, 1980), who explored the phase diagram within mean field theory, and of Hornreich *et al* (1979) who initiated a Monte Carlo study which was extended and refined by Selke and Fisher (1980). Other investigations, some of which will be discussed in more detail below, have been carried out by Fisher and Selke (1979, 1981), Huse *et al* (1981), Villain and Gordon (1980), Rujan (1981), Villain and Bak (1981), Barber and Duxbury (1981a, b), Peschel and Emery (1981), Selke (1981), Williams *et al* (1981), Pesch and Kroemer (1981). The phase diagram which has emerged from this work is depicted in figure 1(a), where the upper Lifshitz point remains controversial (see § 5).

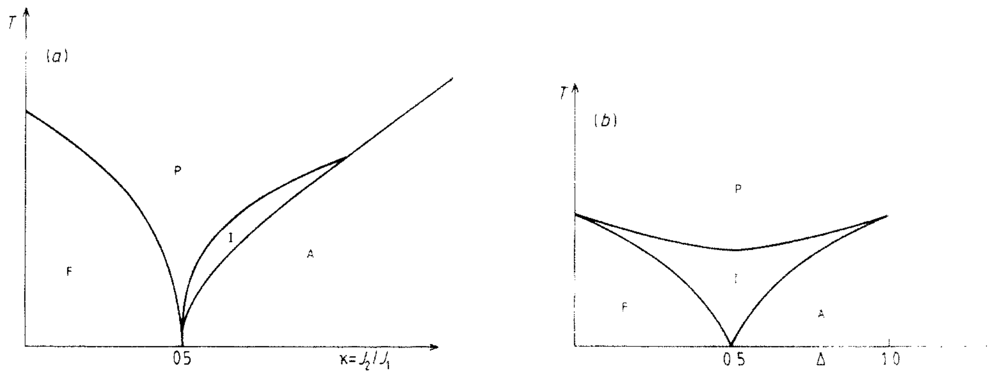


Figure 1. (a) Schematic phase diagram of the $d=2$ ANNNI model: F: ferromagnetically ordered phase, A: antiphase of alternating $++--\ldots$ columns, P: paramagnetic and I: incommensurately modulated (floating phase). (b) Schematic phase diagram of $d=2$, 4ASC model: F: ferromagnetic phase, A: antiferromagnetic phase; columns alternatively $n_i = 0, 1, 2, 3, 0, 1, 2, \ldots$, P: paramagnetic and I: incommensurate phase.

The other class of simple models exhibiting incommensurate/commensurate transitions are the asymmetric p-state clock models ($p \geq 3$) introduced recently by Ostlund (1981) and studied subsequently by Cardy (1981), Huse (1981) and Yeomans and Fisher (1981). The Hamiltonian of the p-state asymmetric clock model (henceforth denoted the pASC model) is given by

$$H = -J \sum_{\langle i,j \rangle} \cos[2\pi(n_i - n_j - \boldsymbol{r}_{ij} \cdot \boldsymbol{\Delta})/p], \tag{1.2}$$

where the sum is now over the *bonds* of a square lattice, p is an integer and the integers n_i and n_j range between 0 and $p-1$. The vector $\boldsymbol{r}_{ij}$ is the unit vector between sites i and j and we shall follow Ostlund and take $\boldsymbol{\Delta} = \Delta \boldsymbol{e}_x$, along the x axis. (Arbitrary $\boldsymbol{\Delta}$ has been considered by Cardy (1981).) For $\Delta = 0$, equation (1.2) reduces to the Hamiltonian of the conventional clock or Z_p-models studied by several authors (see e.g. José *et al* 1977, Elitzur *et al* 1979, Cardy 1980). In this paper, we shall be concerned only with the

† The three-dimensional ANNNI model differs from (1.1) only in the nearest-neighbour interaction now being along the bonds of a simple cubic lattice—the antiferromagnetic interaction remains axial, along one of the spatial axes.

four-state asymmetric clock (4ASC) model, which for $\Delta = 0$ reduces to two independent Ising models. The phase diagram suggested by Ostlund (1981) for this model is shown schematically in figure 1(*b*).

The main aim of this paper is to enquire to what extent the behaviour of these models can be inferred from an analysis of their perturbation expansions about limits at which they reduce to simple Ising models. These limits are for the 4ASC model (as noted above) $\Delta = 0$ and for the ANNNI model (i) $J_2 = 0$ and (ii) $J_1 = 0$.

This approach was suggested by similar analyses of the eight-vertex model (Kadanoff and Wegner 1971), Ashkin–Teller model (Zittartz 1981a) and the square-lattice Ising model with competing nearest- and (diagonal) next-nearest-neighbour interactions (the NN/NNN model) (Barber 1979). In all three examples, the known or expected critical behaviour could be inferred from the lowest non-trivial order of the perturbation expansions of their free energies about the points at which the models decoupled into simple Ising models. These successes suggest that a similar analysis of the ANNNI and 4ASC models could be informative. The essential features which emerge from the analysis can be summarised as follows.

To first order in J_2 at fixed J_1, J_0, we obtain, as expected, an Ising line, the critical temperature of which accords well with that of Monte Carlo calculations (Selke and Fisher 1980, Selke 1981) and (in a highly anisotropic limit) with the quantum Hamiltonian results of Barber and Duxbury (1981a, b). On the other hand, this analysis shows that the phase boundary obtained (Hornreich *et al* 1979) from a Müller-Hartmann–Zittartz (1977) style approximation for the interfacial tension is not exact.

Less expected is the behaviour we infer for small J_1. Here the second-order perturbation expansion is reproduced by a free energy of the form

$$-\beta f(J_0, J_1, J_2) \approx -\tfrac{1}{2}A'[\dot{t}^{2-\alpha(w)}Q(w^4/\dot{t}^{\phi(w)}) - \dot{t}^2]/\alpha(w), \tag{1.3}$$

where A' is the amplitude of the specific heat for $J_1 = 0$,

$$w = \tanh \beta J_1, \tag{1.4}$$

$$\alpha = aw^2 + \mathrm{O}(w^3), \tag{1.5}$$

with the coefficient a depending on J_0 and J_2,

$$\phi = 2 - \alpha - \tfrac{1}{2} = \tfrac{3}{2} + \mathrm{O}(w^2) \tag{1.6}$$

and

$$\dot{t} = [T - T_c(w)]/T_c(0) = [T - T_c(0)]/T_c(0) + \mathrm{O}(w^2), \tag{1.7}$$

with $T_c(w)$ the critical temperature at finite J_1. As $z \to 0$, the scaling function $Q(z)$ behaves as

$$Q(z) = 1 + Q_1 z + \mathrm{O}(z^2). \tag{1.8}$$

If (1.3) is indeed an exact representation of the free energy for arbitrary J_1, it has some interesting implications. Equation (1.6) implies that J_1 is a relevant variable, presumably driving the system to a critical behaviour distinct from the Ising behaviour occurring when $J_1 = 0$. On the other hand, (1.3) suggests that for

$$t \gg w^{4/\phi} \sim J_1^{8/3} \tag{1.9}$$

the ANNNI model should exhibit an effective critical behaviour characterised by non-universal 'effective' exponents, only crossing over to the true critical behaviour for $t \lesssim J_1^{8/3}$. The nature of this behaviour and the key question whether or not this behaviour is the result of a transition to a floating incommensurately modulated phase is, of course, not answered by (1.3) in the absence of any knowledge of the behaviour of $Q(z)$ for large z, i.e. $T \to T_c(w)$ at fixed w.

However, an identical analysis of the 4ASC model yields the same conclusion: the second-order perturbation expansion is reproduced by (1.3) with now $w = O(\Delta)$, Δ being the asymmetry parameter. Indeed, (1.1) can be rewritten in a form (see § 4) that is remarkably similar to the Hamiltonian of the 4ASC model when written in spin variables.

These considerations lead us to conclude that *if either the 4ASC model has a floating phase for arbitrarily small asymmetry or the ANNNI model has a floating phase for arbitrarily large $\kappa = J_2/J_1$ then the other must.* Unfortunately, as is apparent from figure 1 and as we discuss in more detail in § 5, the existing evidence for the extent of a floating phase in these models is both conflicting and inconclusive.

The remainder of the paper is arranged as follows. In the next section, we discuss the limit $J_2 \to 0$ of the ANNNI model which is relatively straightforward. The more complex and interesting limit $J_1 \to 0$ is treated in § 3. In § 4, we formulate the 4ASC model in spin language to reveal its similarity with the ANNNI model. The perturbation expansion of this model to second order in the asymmetry is also discussed in § 4. A concluding discussion in § 5 draws the various threads together and incorporates our results with other recent work on these models. Several technical and more mathematical aspects are relegated to several appendices.

2. ANNNI model for small J_2

2.1. *First-order perturbation expansion*

We consider first the expansion of the free energy of the ANNNI model for small next-nearest-neighbour interaction, J_2. Thus we decompose (1.1) as

$$H = H_0 + V, \tag{2.1}$$

where

$$H_0 = -\sum_{(i,j)} (J_1 s_{i,j} s_{i+1,j} + J_0 s_{ij} s_{i,j+1}) \tag{2.2}$$

is the Hamiltonian of the anisotropic nearest-neighbour Ising model on a square lattice and

$$V = J_2 \sum_{(i,j)} s_{i,j} s_{i+2,j}. \tag{2.3}$$

We can then write the partition function

$$Z_N = \sum_{\{s_{i,j}=\pm 1\}} e^{-\beta H} = \Bigg(\sum_{\{s_{i,j}=\pm 1\}} \exp(-\beta H_0)\Bigg) \langle e^{-\beta V} \rangle_0, \tag{2.4}$$

where $\langle \cdot \rangle_0$ denotes an ensemble average with respect to H_0. On expanding

$$\begin{aligned} e^{-\beta V} &= (\cosh K_2)^N \prod_{(i,j)} (1 - w_2 s_{i,j} s_{i+2,j}) \\ &= (\cosh K_2)^N \Big(1 - w_2 \sum_{(i,j)} s_{i,j} s_{i+2,j} + O(w_2^2)\Big) \end{aligned} \tag{2.5}$$

where N is the total number of sites and

$$w_2 = \tanh \beta J_2, \tag{2.6}$$

the required expansion of the free energy (with $K_i = \beta J_i > 0$, $i = 0, 1, 2$)

$$-\beta f(K_0, K_1, K_2) = \lim_{N\to\infty} \left(\frac{1}{N} \ln Z_N\right) \tag{2.7}$$

follows immediately. Explicitly we obtain

$$\beta f(K_0, K_1, K_2) = \beta f_0(K_0, K_1) - \ln(\cosh K_2) + w_2 \Gamma_0(2, 0) + O(w_2^2), \tag{2.8}$$

where the leading term is the Onsager (1944) free energy of (2.2) and the coefficient of w_2,

$$\Gamma_0(2, 0) = \langle s_{0,0} s_{2,0} \rangle_0, \tag{2.9}$$

is the next-nearest-neighbour correlation function of (2.2) in the x direction. This is known for arbitrary K_0 and K_1 (see e.g. McCoy and Wu 1973) and can be expressed as a (2×2) determinant whose elements are given by elliptic integrals. These results allow, in principle, the determination of the shift in the critical temperature to first order in J_2 for arbitrary J_0 and J_1. We shall however restrict our discussion to two cases: isotropic nearest-neighbour interactions ($J_0 = J_1$) for which there is Monte Carlo data (Selke and Fisher 1980, Selke 1981) and series results (Redner unpublished) and the highly anisotropic limit relevant to the quantum Hamiltonian formulation of Barber and Duxbury (1981a).

2.2. Shift in T_c—isotropic nearest-neighbour interactions

To determine the effect of non-zero K_2 on the critical behaviour we expand the singular point of (2.8) (with $K_0 = K_1 = K$) near the critical temperature K_c given by

$$\sinh 2K_c = 1. \tag{2.10}$$

The leading-order term behaves as (Onsager 1944)

$$\beta f_0(K) = A(\Delta K)^2 \ln|\Delta K| + \dots \tag{2.11}$$

as $\Delta K = K_c - K \to 0$ and $A = 4/\pi$, while $\Gamma_0(2, 0)$ has the expansion (Fisher and Burford 1967)

$$\Gamma_0(2, 0) = (1 - 4/\pi^2) + (16\sqrt{2}/\pi^2)\Delta K \ln|\Delta K| + O(\Delta K). \tag{2.12}$$

Hence the singular part of (2.8) behaves for small ΔK as

$$\beta f_s(K_0=K, K_1=K, K_2) \approx A(\Delta K)^2 \ln|\Delta K| + w_2(16\sqrt{2}/\pi^2)\Delta K \ln|\Delta K| + \dots \tag{2.13}$$

The corrections here are either $O(w_2^2)$ or $o(\Delta K \ln \Delta K)$, all non-singular terms being absorbed into the regular part of the free energy. The expansion (2.13) is consistent with the expansion to first order in w_2 of

$$\beta f_s(K, K, K_2) = A(\Delta \dot{K})^2 \ln|\Delta \dot{K}| + O(\Delta \dot{K}^2) \tag{2.14}$$

with

$$\Delta \dot{K} = \Delta K + 2\sqrt{2} w_2/\pi + O(w_2^2). \tag{2.15}$$

Equation (2.14) thus shows that to first order in K_2, the ANNNI model continues to exhibit Ising-like behaviour (e.g. a logarithmically divergent specific heat) at a shifted critical temperature $T_c(J_2)$. Setting $\Delta \dot{K} = 0$ in (2.15) gives

$$K_c(w_2) = K_c(0) + 2\sqrt{2} w_2/\pi + O(w_2^2), \tag{2.16}$$

from which it follows that

$$T_c(\kappa) = T_c(0)[1 - (2\sqrt{2}/\pi)\kappa + O(\kappa^2)] \tag{2.17}$$

where

$$\kappa = J_2/J_1. \tag{2.18}$$

Hornreich *et al* (1979) have calculated the phase boundary of ferromagnetic states of the ANNNI model by the method of Müller-Hartmann and Zittartz (1977). In this approach, one considers the fluctuations (suitably restricted) of the interface between two oppositely aligned phases and derives an approximation for the interfacial tension. The expression for the phase boundary,

$$\sinh[2(K_1 - 2K_2)] \sinh 2K_0 = 1, \tag{2.19}$$

follows from the temperature at which the resulting interfacial free energy vanishes. Selke and Fisher (1980) found that (2.19) was in reasonable agreement with their Monte Carlo results for $0 \leqslant J_2/J_1 \leqslant 0.4$, although some systematic deviation occurred for larger values.

Setting $J_1 = J_0$, we can easily expand (2.15) to first order in κ, to obtain

$$T_c(\kappa) = T_c(0)[1 - \kappa + O(\kappa^2)]. \tag{2.20}$$

Comparison of the result with (2.17) shows that despite the Monte Carlo agreement the Müller-Hartmann–Zittartz result is only approximate except at $\kappa = 0$. The accuracy of the Monte Carlo results is however insufficient to differentiate between (2.19) and (2.20), the error in the coefficient of κ being about 10%. This error is comparable to that found in other failures of the Müller-Hartmann–Zittartz approximation (see e.g. Burkhardt 1978, Baxter and Tsang 1980, Baxter *et al* 1980, Zittartz 1980, 1981b).

2.3. Shift in critical coupling—quantum Hamiltonian limit

The analogies between statistical mechanics and quantum field theory (see e.g. Kogut 1979) have been extensively exploited in recent years. In the case of the ANNNI model, Barber and Duxbury (1981a) (see also Rujan 1981) have shown that in the anisotropic limit

$$J_0 \to \infty, \qquad J_2 = \kappa J_1 \to 0, \qquad \lambda = \beta J_1 \exp(2\beta J_0) = O(1), \tag{2.21}$$

the phase diagram can be explored by studying the ground state of the quantum Hamiltonian

$$H=-\sum_m \sigma_m^x-\lambda\sum_m\left(\sigma_m^z\sigma_{m+1}^z-\kappa\sigma_m^z\sigma_{m+2}^z\right). \tag{2.22}$$

Here the spatial dimension (corresponding to the x direction of the original ANNNI model (1.1)) is a discrete chain but time (corresponding to the y direction in (1.1)) is continuous, the limit (2.21) effectively forcing the lattice spacing in the y direction to zero (see Fradkin and Susskind 1978, Kogut 1979). The σ's appearing in (2.22) are Pauli matrices and λ plays the role of temperature ($\lambda\propto 1/T$). The ground state energy of (2.22) is now equal to the free energy of the ANNNI model in the limit (2.21). Assuming that this limit does not change the universality class of the Hamiltonian, universal parameters, such as critical exponents, then follow from the singularities of the ground state energy of (2.22) as a function of λ. This was the approach adopted by Barber and Duxbury (1981a, b), who constructed Rayleigh–Schrödinger perturbation expansions about the trivial limits $\lambda=0$ and $\lambda=\infty$ for various physical quantities and then analysed these expansions by standard series methods.

In the limit $\kappa=0$, (2.22) reduces to the one-dimensional transverse Ising model, which has been diagonalised analytically by Pfeuty (1970). This suggests that the behaviour for small κ can be explored by perturbing about this point. To first order, standard Rayleigh–Schrödinger perturbation theory yields for the ground state energy per spin

$$E_0(\lambda,\kappa)=E_0^{(0)}(\lambda)+\lambda\kappa\langle\sigma_m^z\sigma_{m+2}^z\rangle_0+\mathrm{O}(\kappa^2), \tag{2.23}$$

where $\langle\cdot\rangle_0$ denotes an expectation value over the unperturbed ($\kappa=0$) ground state. From Pfeuty's results we immediately have

$$E_0^{(0)}(\lambda)=-\frac{2}{\pi}\int_0^\pi(1+\lambda^2+2\lambda\cos\theta)^{1/2}\,\mathrm{d}\theta, \tag{2.24}$$

and

$$\langle\sigma_m^z\sigma_{m+2}^z\rangle_0=\begin{vmatrix}G(-1) & G(-2)\\ G(0) & G(-1)\end{vmatrix}, \tag{2.25}$$

with

$$G(n)=L(n)+\lambda L(n+1), \tag{2.26}$$

$$L(n)=\frac{1}{\pi}\int_0^\pi\frac{\mathrm{d}\theta\cos n\theta}{(1+\lambda^2+2\cos\theta)^{1/2}}. \tag{2.27}$$

The integrals appearing in (2.24) and (2.27) can be expressed as elliptic integrals, from which it follows that the singular part of $E_0^0(\lambda)$ is

$$E_{0,s}^{(0)}(\lambda)=(2\pi)^{-1}(1-\lambda)^2\ln|1-\lambda|+\mathrm{O}[(1-\lambda)^2] \tag{2.28}$$

and

$$\langle\sigma_m^z\sigma_{m+2}^z\rangle_0=(16/3\pi^2)[1+(1-\lambda)\ln|1-\lambda|+\mathrm{O}(1-\lambda)] \tag{2.29}$$

as $\lambda\to 1$. This analysis is summarised in appendix 1. Comparison of these results with (2.11) and (2.12) confirms that the singularity structure of the ground state of the transverse Ising model (equation (2.22) with $\kappa=0$) is identical to that of the conventional Ising model.

We may now proceed as in § 2.2. Substituting (2.28) and (2.29) in (2.23), we find that the resulting expression for the singular part, $E_{0,s}(\lambda, \kappa)$, of the ground state energy is consistent with the expansion to $O(\kappa)$ of

$$E_{0,s}(\lambda, \kappa) \simeq (2\pi)^{-1}(\Delta\dot{\lambda})^2 \ln|\Delta\dot{\lambda}| + O(\Delta\dot{\lambda}^2) \tag{2.30}$$

with

$$\Delta\dot{\lambda} = 1 - \lambda + 16\kappa/3\pi + O(\kappa^2) \tag{2.31}$$

so that

$$1/\lambda_c = 1 - 16\kappa/3\pi + O(\kappa^2) \tag{2.32}$$

which is the analogue of (2.17).

The result (2.32) for the shift in the critical coupling may again be compared with that given by the Müller-Hartmann–Zittartz approximation (2.19), which in the limit (2.21) reduces to

$$1/\lambda_c = 1 - 2\kappa. \tag{2.33}$$

Since $16/3\pi = 1.699\ldots$, we note that the Müller-Hartmann–Zittartz result is again in error at first order in κ.

We may also compare (2.32) with the phase boundary determined by Barber and Duxbury (1981b) from analysis of various weak-coupling perturbation expansions in $1/\lambda$. This comparison is shown in figure 1, (2.32) being seen to be a very accurate representation of the numerical data for small κ, whereas (2.33) lies outside the error bars. On the other hand, (2.33) appears (Villain and Bak 1981, Rujan 1981) to be asymptotically exact as $\kappa \to \frac{1}{2}$, where T_c and $1/\lambda_c$ vanish. A simple approximant, which satisfies (2.32) as $\kappa \to 0$ and (2.33) as $\kappa \to \frac{1}{2}$, is

$$\frac{1}{\lambda_c} = \frac{1 - 2\kappa}{1 - 2(1 - 8/3\pi)\kappa(1 - 2\kappa)}. \tag{2.34}$$

As shown in figure 2, this result affords a rather accurate representation of the numerical results over the whole range $0 \leqslant \kappa \leqslant \frac{1}{2}$.

3. ANNNI model for small J_1

We now turn to the expansion of the free energy of the ANNNI model for small nearest-neighbour interaction J_1, i.e. $\kappa = J_2/J_1 \gg 1$. In this limit it is convenient to divide the lattice into two sublattices Ω_σ and Ω_τ and label the sites as indicated in figure 3. We denote the spins Ω_σ and Ω_τ by σ and τ respectively; in terms of the original spins $s_{i,j}$,

$$\sigma_{i,j} = s_{2i,j}, \qquad \tau_{i,j} = s_{2i+1,j}. \tag{3.1}$$

The Hamiltonian (1.1) can now be decomposed as

$$H\{\sigma, \tau\} = H_0\{\sigma\} + H_0\{\tau\} + V\{\sigma, \tau\}, \tag{3.2}$$

where

$$H_0\{\sigma\} = -\sum_{(i,j)\in\Omega_\sigma} (J_0\sigma_{i,j}\sigma_{i,j+1} - J_2\sigma_{i,j}\sigma_{i+1,j}), \tag{3.3}$$

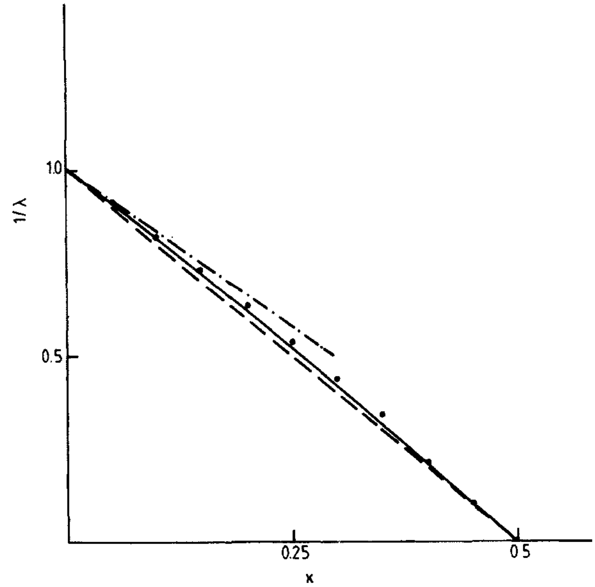


Figure 2. Ferromagnetic phase boundary of the ANNNI Hamiltonian (2.22) ground state. The full dots (•) are the results of analysis of weak-coupling expansions (Barber and Duxbury 1981a, b), the error bars being smaller than the size of the dots. The lines depict: —— the approximant (2.34), - - - the Müller-Hartmann–Zittartz result (2.33) and – · – the first-order perturbative calculation (2.32) about $\kappa = 0$.

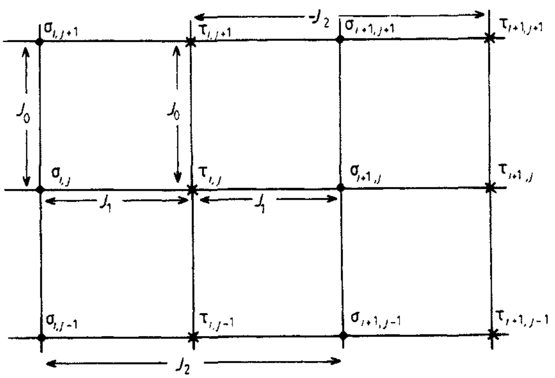


Figure 3. Sublattices Ω_σ and Ω_τ (see text) of the ANNNI model.

$$H_0\{\tau\} = -\sum_{(i,j)\in\Omega_\tau} (J_0\tau_{i,j}\tau_{i,j+1} - J_2\tau_{i,j}\tau_{i+1,j}), \tag{3.4}$$

$$V\{\sigma,\tau\} = -J_1 \sum_{(i,j)\in\Omega_\sigma} \sigma_{i,j}(\tau_{i-1,j} + \tau_{i,j}). \tag{3.5}$$

3.1. *The unperturbed system* ($J_2 = 0$)

For $J_1 = 0$, the system decouples into two nearest-neighbour Ising models (one on Ω_σ, the other on Ω_τ). Each of these models has antiferromagnetic interactions ($-J_2$)

horizontally and ferromagnetic interactions (J_0) vertically†. The partition functions for both lattices can now be expressed in terms of that of an anisotropic *ferromagnetic* nearest-neighbour model by making the transformation

$$\sigma_{i,j} \to \sigma'_{i,j} = (-)^i \sigma_{i,j}, \qquad \tau_{i,j} \to \tau'_{i,j} = (-)^i \tau_{i,j}. \tag{3.6}$$

Clearly the new spins σ' and τ' are again Ising spins. Thus the partition function of the σ spins

$$\begin{aligned}\sum_{\{\sigma=\pm 1\}} \exp(-\beta H_0) &= \sum_{\{\sigma=\pm 1\}} \exp\Big(\sum_{(i,j)\in\Omega_\sigma} (K_0\sigma_{i,j}\sigma_{i,j+1} - K_2\sigma_{i,j}\sigma_{i+1,j})\Big)\\ &= \sum_{\{\sigma'=\pm 1\}} \exp\Big(\sum_{(i,j)\in\Omega_\sigma} (K_0\sigma'_{i,j}\sigma'_{i,j+1} + K_2\sigma'_{i,j}\sigma'_{i+1,j})\Big)\\ &= Z^{(0)}_{N/2}(K_0, K_2).\end{aligned} \tag{3.7}$$

Here $Z^{(0)}_{N/2}(K_0, K_2)$ denotes the Onsager (1944) result for the partition function of a square lattice Ising model of $\frac{1}{2}N$ sites with anisotropic ferromagnetic interactions J_0 and J_2 in the y and x directions respectively. An identical result holds for the τ lattice.

Thus for $J_1 = 0$, the ANNNI model (1.1) exhibits a conventional Ising singularity at $\beta = \beta_c$ determined by

$$\sinh 2\beta_c J_0 \sinh 2\beta_c J_2 = 1. \tag{3.8}$$

Specifically, the singular part of the free energy varies (generalising (2.11)) as

$$\beta f_s(K_1 = 0, K_0, K_2) \approx A(J_0, J_2)t^2 \ln|t| \ldots \tag{3.9}$$

as $t \to 0$, where $t = (1 - \beta_c/\beta) \propto (T - T_c)$.

3.2. *Expansion to $O(J_1^2)$*

To consider the effect of non-zero J_1 on the critical behaviour, we now expand the partition function of (3.2),

$$Z_N(K_0, K_1, K_2) = \sum_{\{\sigma=\pm 1\}} \sum_{\{\tau=\pm 1\}} \exp(-\beta H\{\sigma, \tau\}), \tag{3.10}$$

to second order in K_1, where $K_i = \beta J_i \geq 0$. It is again convenient to apply the transformation (3.6) so that the unperturbed Hamiltonian is completely ferromagnetic. The perturbation V then becomes

$$V\{\sigma, \tau\} = -J_1 \sum_{(i,j)\in\Omega_\sigma} \sigma'_{i,j}(\tau'_{i,j} - \tau'_{i-1,j}). \tag{3.11}$$

Defining

$$w_1 = \tanh \beta J_1, \tag{3.12}$$

we have

$$\exp(-\beta V) = (\cosh K_1)[1 + w_1 U + w_1^2 U_2 + O(w_1^3)], \tag{3.13}$$

† The fact that Ω_σ and Ω_τ are rectangular rather than square has no effect on the subsequent argument, the lattice parameters not entering the thermodynamic quantities.

where

$$U_1 = \sum_{(i,j)\in\Omega_\sigma} \sigma'_{i,j}(\tau'_{ij} - \tau'_{i-1,j}) \tag{3.14}$$

$$U_2 = -\sum_{(i,j)\in\Omega_\sigma} \tau'_{i,j}\tau'_{i-1,j} + \sum_{(i,j)\in\Omega_\sigma} \sum_{\substack{(k,l)\in\Omega_\sigma \\ (i,j)\neq(k,l)}} \sigma'_{i,j}\sigma'_{k,l}(\tau'_{i,j} - \tau'_{i-1,j})(\tau'_{k,l} - \tau'_{k-1,l}). \tag{3.15}$$

Thus

$$\begin{aligned} Z_N(K_0, K_1, K_2) &= [Z^{(0)}_{N/2}(K_0, K_2)]^2 \langle \exp(-\beta V)\rangle_0 \\ &= (\cosh K_1)^N [Z^{(0)}_{N/2}(K_0, K_2)]^2 [1 + w_1\langle U_1\rangle_0 + w_1^2 \langle U_2\rangle_0 + \mathrm{O}(w_1^3)], \end{aligned} \tag{3.16}$$

where $\langle\cdot\rangle_0$ denotes an expectation value with respect to the unperturbed Hamiltonian, $H_{0,T} = H'_0\{\sigma'\} + H'_0\{\tau'\}$, where $H'_0\{\sigma'\}$ and $H'_0\{\tau'\}$ are given by (3.3) and (3.4) respectively with J_2 replaced by $-J_2$. Thus in calculating $\langle U_1\rangle_0$ and $\langle U_2\rangle_0$ the products of σ' and τ' spins decouple and can be expressed in terms of correlation functions of the *ferromagnetic* Ising Hamiltonians $H'_0\{\sigma'\}$ and $H'_0\{\tau'\}$.

The expectation value of U_1 vanishes even† for $T < T_c$, while some algebra reduces $\langle U_2\rangle_0$ to

$$\langle U_2\rangle_0 = -N + \tfrac{1}{2}N\Gamma_0(1, 0) + N\Phi(K_0, K_2), \tag{3.17}$$

where

$$\Gamma_0(i, j) = \langle \sigma'_{0,0}\sigma'_{i,j}\rangle_0 = \langle \tau'_{0,0}\tau'_{i,j}\rangle_0 \tag{3.18}$$

is the pair correlation function of the ferromagnetic anisotropic nearest-neighbour Ising models $H'_0\{\sigma'\}$ and $H'_0\{\tau'\}$. The function

$$\Phi(K_0, K_2) = \sum_{(k,l)\in\Omega_\sigma} \Gamma_0(k, l)\Delta\Gamma_0(k, l), \tag{3.19}$$

where Δ is a lattice difference operator defined by

$$\Delta g(i, j) = g(i, j) - \tfrac{1}{2}g(i-1, j) - \tfrac{1}{2}g(i+1, j). \tag{3.20}$$

Substituting (3.17) in (3.16) yields the required expansion of the free energy per spin

$$\begin{aligned} &\beta f(K_0, K_1, K_2) \\ &\quad = \lim_{N\to\infty}\left(-\frac{1}{N}\ln Z_N\right) \\ &\quad = \beta f^{(0)}(K_0, K_2) - \cosh K_1 + w_1^2(1 - \tfrac{1}{2}\Gamma(1, 0) - \Phi(K_0, K_2)) + \mathrm{O}(w_1^3) \end{aligned} \tag{3.21}$$

where $\beta f^{(0)}(K_0, K_2)$ is the Onsager free energy for anisotropic nearest-neighbour couplings K_0 and K_2.

Expanding (3.20) in the lattice spacing $(2a)$ of the lattice Ω_σ in the x direction allows Δ to be approximated by

$$\Delta = -2a^2\partial^2/\partial x^2 + \mathrm{O}(a^4). \tag{3.22}$$

The integral test can then be used to show that the sum in (3.19) converges even at the critical temperature where $\Gamma_0(k, l) \sim R^{-1/4}$ with R an appropriately scaled distance of (k, l) from the origin (see (3.25)).

† Strictly speaking, for $T < T_c$, the expectation values should be calculated for a finite value of an appropriate symmetry breaking field which is then taken to zero.

3.3. Analysis near criticality

We now investigate the behaviour of the singular part of (3.21) near the critical temperature β_c of the unperturbed system, ($J_1 = 0$), where β_c is given by (3.8). The significant feature of (3.21) is the *quadratic* dependence of the function $\Phi(K_0, K_2)$ on the pair correlation function Γ_0. Now,

$$\Gamma_0(i,j) = \Gamma_{0,c}(i,j) - E(i,j)t\ln|t| \ldots, \qquad t \to 0, \tag{3.23}$$

for all (i, j) (Fisher and Burford 1967, Wu *et al* 1976). Thus we expect Φ to contain terms involving $t\ln|t|$ and $t^2(\ln|t|)^2$, which can be indicative of a marginal operator (Kadanoff and Wegner 1971). However, some care is required in explicitly evaluating the coefficients, since (Wu *et al* 1976)

$$E(i,j) \sim R_{ij}^{3/4}, \qquad R_{ij} \to \infty, \tag{3.24}$$

where

$$R_{ij} = \left[\left(\frac{\sinh 2K_0}{\sinh 2K_2}\right)^{1/2} i^2 + \left(\frac{\sinh 2K_2}{\sinh 2K_0}\right)^{1/2} j^2\right]^{1/2} \tag{3.25}$$

is an appropriate radial measure of distance. Thus a direct substitution of (3.23) into (3.19) leads to divergent sums.

To analyse Φ in the limit $\beta \to \beta_c$, we write

$$\Phi = \Phi_< + \Phi_>, \tag{3.26}$$

where $\Phi_<$ ($\Phi_>$) is defined by (3.19) but with the sum restricted to lattice sites (k, l) inside (outside) the elliptical region

$$\mathcal{R} = \{(k,l)|R_{kl} \leq r_0\}. \tag{3.27}$$

Since the sum $\Phi_<$ is now a finite sum, we can substitute (3.23) directly to obtain

$$\Phi_< = \Phi_{<,c} - p_< t\ln|t| + q_<(t\ln|t|)^2 \ldots, \tag{3.28}$$

where

$$\Phi_{<,c} = \sum_{(k,l)\in\mathcal{R}} \Gamma_{0,c}(k,l)\Delta\Gamma_{0,c}(k,l), \tag{3.29}$$

$$p_< = \sum_{(k,l)\in\mathcal{R}} [\Gamma_{0,c}(k,l)\Delta E(k,l) - E(k,l)\Delta\Gamma_0(k,l)], \tag{3.30}$$

$$q_< = \sum_{(k,l)\in\mathcal{R}} E(k,l)\Delta E(k,l). \tag{3.31}$$

The sum $\Phi_>$ requires more care. We assume that (i) $r_0 \gg a$, the lattice spacing, and (ii) $t \ll 1$, so we can replace $\Gamma(k, l)$ by its scaling form (Wu *et al* 1976)

$$\Gamma(k,l) \approx t^{1/4}F(Rt). \tag{3.32}$$

The sum can now be replaced by an integral with Δ approximated by (3.22). This yields

$$\Phi_> \approx -t^{1/2} \iint_{(x,y)\notin\mathcal{R}} \mathrm{d}x\mathrm{d}y\, F(Rt)\frac{\partial^2}{\partial x^2}[F(Rt)]. \tag{3.33}$$

The region $\mathcal{R}$ can be mapped into a circle by the change of variables

$$X = \lambda^{1/2}x, \qquad Y = y/\lambda^{1/2}, \tag{3.34}$$

where

$$\lambda = (\sinh 2K_0/\sinh 2K_2)^{1/2}. \tag{3.35}$$

Under this transformation the integral in (3.33) reduces to

$$\Phi_> \simeq -2\pi\lambda t^{1/2} \int_{r_0}^{\infty} R \, \mathrm{d}R \, F(Rt) \frac{\partial^2}{\partial X^2} F(Rt) \tag{3.36}$$

with $R^2 = X^2 + Y^2$. The integral is now symmetric in X and Y. Thus we can replace $\partial^2/\partial X^2$ by

$$\tfrac{1}{2}\nabla^2 = \frac{1}{2}\left(\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2}\right) = \frac{1}{2R}\frac{\mathrm{d}}{\mathrm{d}R} R \frac{\mathrm{d}}{\mathrm{d}R}. \tag{3.37}$$

Finally, defining

$$\rho = tR, \tag{3.38}$$

we obtain

$$\Phi_> \approx -\pi\lambda t^{1/2} G(tr_0), \tag{3.39}$$

where

$$G(z) = \int_z^{\infty} F(\rho) \frac{\mathrm{d}}{\mathrm{d}\rho}\left(\rho \frac{\mathrm{d}F}{\mathrm{d}\rho}\right) \mathrm{d}\rho. \tag{3.40}$$

In appendix 2, we show that

$$G(z) = g_0 z^{-1/2}[1 - \hat{Q}_0 z^{1/2} - 5z(\ln z + \gamma) + \tfrac{3}{4}(z \ln z)^2 + \mathrm{O}(z^2 \ln z)] \tag{3.41}$$

as $z \to 0$, where g_0, $\hat{Q}_0$ and γ are constants (depending on J_0 and J_2). Substituting this result in (3.39) and combining with (3.28) yields

$$\Phi(K_0, K_2) = \Phi_c + 2\pi\lambda Q_0|t|^{1/2} - pt \ln|t| - p't + qt^2(\ln|t|)^2 + \mathrm{O}(t^2 \ln|t|). \tag{3.42}$$

The coefficients in this expansion are functions of J_0 and J_2, explicit formulae for the coefficients g_0, $\hat{Q}_0$ and γ in (3.41) being given by (A2.23)–(A2.25), with Q_0 given explicitly in (A2.21).

The required expansion of the singular part of $f(K_0, K_1, K_2)$ for β near $\beta_c = \beta_c(K_0, K_2)$ now follows on substituting (3.42), (3.23), together with (3.9), in (3.21). This gives

$$\begin{aligned}\beta f_s(K_0, K_1, K_2) &\approx A(J_0, J_2)t^2 \ln|t| + w_1^2\{2\pi\lambda Q_0|t|^{1/2} \\ &\quad + [p + \tfrac{1}{2}E(1, 0)]t \ln|t| - qt^2(\ln|t|)^2\} + \ldots, \qquad t \to 0.\end{aligned} \tag{3.43}$$

The correction terms in this expansion are $\mathrm{O}(t^3 \ln t)$ from $f_s^{(0)}$ and $\mathrm{O}(w_1^2 t^2 \ln t)$ from Φ. In addition, all non-singular terms have been absorbed into the regular part of $f(K_0, K_1, K_2)$.

The significant feature of the expansion (3.43) is the presence of powers of $\ln|t|$. It was a similar occurrence of such factors in their perturbation expansion of the free energy of the eight-vertex model that led Kadanoff and Wegner (1971) to argue that they are indications of a marginal operator. The perturbation expansions of the NN/NNN model (Barber 1979) and the Ashkin–Teller model (Zittartz 1981a) also exhibit such factors, again suggesting marginal behaviour. The existence of a marginal operator, in turn, implies the possibility of non-universal behaviour. However, (3.43) differs significantly from the expansions found in these earlier calculations by the presence of a term of order $w_1^2 t^{1/2}$. If this was absent, the logarithmic terms could be simply re-exponentiated to give a non-universal line along which the singular part varies as $t^{2-\alpha}$ with α a function of K_0, K_1, K_2.

3.4. *Scaling form*

To account for the term in (3.43) of order $w_1^2 t^{1/2}$ we need a more complex form for the free energy than that implied simply by a non-universal specific heat exponent. However, any attempt to guess one solely on the basis of (3.43) must be fairly speculative. Perhaps the most simple ansatz for the free energy, in the light of (3.43), is to write

$$\beta f_s(K_0, K_1, K_2) \approx -A[\dot{t}^{2-\alpha} Q(w_1^4/t^{\phi}) - \dot{t}^2]/\alpha(w_1) \tag{3.44}$$

where

$$Q(z) = 1 + Q_1 z + \mathrm{O}(z^2) \qquad \text{as } z \to 0. \tag{3.45}$$

This reproduces (3.43) in the limit $w_1 \to 0$ if

$$Q_1 = 4\pi\lambda Q_0 q/A^2, \tag{3.46}$$

$$\phi = 2 - \alpha - \tfrac{1}{2}, \tag{3.47}$$

$$\alpha = (2q/A)w_1^2 + \mathrm{O}(w_1^2), \tag{3.48}$$

$$\dot{t} = t + \varepsilon(w_1^2), \tag{3.49}$$

with

$$\varepsilon(w_1^2) = \tfrac{1}{2}w_1^2[p + \tfrac{1}{2}E(1, 0)]/A + \mathrm{O}(w_1^2) \tag{3.50}$$

and A is the unperturbed ($J_1 = 0$) amplitude (recall (3.9)).

Equation (3.48) implies that the critical temperature varies as

$$T_c(J_1) = T_c(0)[1 + \eta J_1^2 + \mathrm{O}(J_1^2)], \tag{3.51}$$

where the coefficient η is a complicated function (which we have not evaluated) of the coupling parameters. A quadratic dependence, such as (3.51), is consistent with the series results of Barber and Duxbury (1981b) and is also predicted by the approximate boundary found by Pesch and Kroemer (1981) using the Müller-Hartmann–Zittartz method. Unfortunately, as noted in the Introduction, (3.44) does not give any information on the behaviour as $T \to T_c(J_1)$, since in this limit the argument $w_1^2/\dot{t}^{\phi}$ tends to infinity. Hence the critical behaviour at finite non-zero J_1 is determined by the asymptotic behaviour of the function $Q(x)$ as $x \to \infty$.

We shall discuss some of the other physical implications of (3.44) further in § 5. Before doing so we show that the 4ASC model for small Δ has a similar perturbation expansion to (3.43).

4. 4ASC model for small Δ

4.1. Spin representation of 4ASC model

We consider the asymmetric clock model (1.2) with $p=4$ and $\boldsymbol{\Delta}=(\Delta, 0)$. We introduce Ising spins σ_i and τ_i via the relations

$$\cos(\tfrac{1}{2}\pi n_i)=\tfrac{1}{2}(\sigma_i-\tau_i), \qquad \sin(\tfrac{1}{2}\pi n_i)=\tfrac{1}{2}(\sigma_i+\tau_i). \tag{4.1}$$

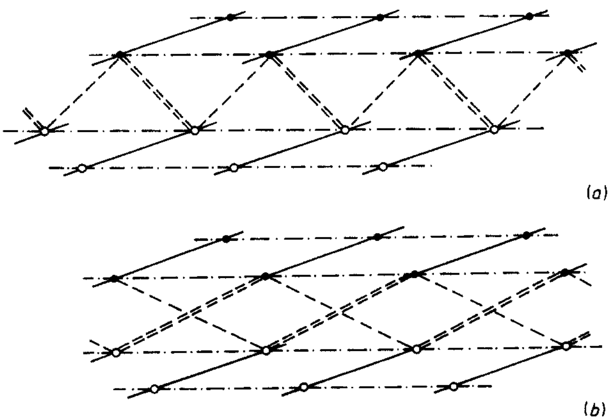
Hence on expanding the cosine in (1.2) we obtain

$$H_{4\mathrm{ASC}}=-\tfrac{1}{2}J\sum_{\langle i,j\rangle}[\cos(\tfrac{1}{2}\pi\Delta e_{ij})(\sigma_i\sigma_j+\tau_i\tau_j)+\sin(\tfrac{1}{2}\pi\Delta e_{ij})(\sigma_i\tau_j-\sigma_j\tau_i)], \tag{4.2}$$

where $e_{ij}=1$ if $\langle i, j\rangle$ is a horizontal bond and zero if $\langle i, j\rangle$ is vertical. It is convenient to label the sites of the lattice by (m, n) and write the sum in (4.2) as a sum over sites, i.e. we write

$$\begin{aligned} H_{4\mathrm{ASC}}=-\tfrac{1}{2}J\sum_{(m,n)}[(\cos\tfrac{1}{2}\pi\Delta)(\sigma_{m,n}\sigma_{m+1,n}+\tau_{m,n}\tau_{m+1,n})\\ +(\sigma_{m,n}\sigma_{m,n+1}+\tau_{m,n}\tau_{m,n+1})+(\sin\tfrac{1}{2}\pi\Delta)\sigma_{m,n}(\tau_{m+1,n}-\tau_{m-1,n})]. \end{aligned} \tag{4.3}$$

This is our required spin-representation of the 4ASC model. For $\Delta=0$ the decoupling into two independent isotropic nearest-neighbour Ising models is apparent. While the spins $\sigma_{m,n}$ and $\tau_{m,n}$ were introduced on the *same* site, it is informative to regard them as populating different lattices and to regard (4.3) as referring to a two-layer geometry as illustrated in figure 4(*b*).



(*a*)

(*b*)

Figure 4. Two-layer representations of (*a*) the ANNNI model (4.4): σ spins (•), τ spins (◦); interactions: $-J_0$ (——), $-J_1$ (- • -), $-J_2$ (– – –), $+J_2$(= = =); (*b*) the 4ASC model (4.3): σ spins (•), τ spins (◦); interactions: $-\tfrac{1}{2}J\cos(\tfrac{1}{2}\pi\Delta)$ (——), $-\tfrac{1}{2}J$ (- • -), $-\tfrac{1}{2}J\sin(\tfrac{1}{2}\pi\Delta)$ (– – –), $+\tfrac{1}{2}J\sin(\tfrac{1}{2}\pi\Delta)$ (= = =).

4.2. Relation to ANNNI *model*

The form (4.3) is rather, but not exactly, similar to the form of the ANNNI model Hamiltonian in the two-lattice representation introduced in the previous section.†

† The ANNNI model can also be regarded as a four-state model (see appendix 3); the spin representations are however more useful for our purposes.

Explicitly from (3.3)–(3.5) we have

$$H_{\text{ANNNI}} = -\sum [J_0(\sigma_{m,n}\sigma_{m,n+1} + \tau_{m,n}\tau_{m,n+1})$$
$$+ J_2(\sigma_{m,n}\sigma_{m+1,n} + \tau_{m,n}\tau_{m+1,n}) - J_1\sigma_{m,n}(\tau_{m,n} - \tau_{m-1,n})], \tag{4.4}$$

where the sum is restricted to one sublattice, say Ω_σ, and we have applied the transformation (3.6). With the correspondence

$$J_0 \leftrightarrow \tfrac{1}{2}J, \qquad J_1 \leftrightarrow \tfrac{1}{2}J \sin \tfrac{1}{2}\Delta\pi, \qquad J_2 \leftrightarrow J \cos \tfrac{1}{2}\Delta\pi, \tag{4.5}$$

(4.4) and (4.3) are remarkably similar. There is however a subtle topological difference due to the σ and τ spins now being on different sites of the original lattice. This difference is most clearly seen if we regard the ANNNI model (4.4) as a two-layer system as shown in figure 4(a). Comparison of figures 4(a) and 4(b) shows that in the ANNNI model the two layers are shifted relative to each other whereas in the 4ASC model the layers are superimposed. This topological difference is reminiscent of that between the eight-vertex and Ashkin–Teller models when regarded as two sublattice (layer) systems. As in that case, this difference must ultimately lead to distinctly different behaviour in the two models. However, to second order in Δ, the perturbation expansions are identical under the correspondence (4.5); only at higher order does the topological distinction become apparent. Thus we can take over the analysis of § 3 and conjecture that the singular part of the free energy of the 4ASC model (with $K = \beta J$) behaves as

$$\beta f_s(K, \Delta) \approx -A[\dot{t}^{2-\alpha}Q(w^4/\dot{t}^{\phi}) - \dot{t}^2]/\alpha(w) \tag{4.6}$$

with

$$w = \tanh\{\tfrac{1}{2}K[\sin(\tfrac{1}{2}\Delta\pi)]\} \approx K\Delta\pi/4 + \mathrm{O}(\Delta^3) \tag{4.7}$$

and the other quantities as defined in (3.45)–(3.50).

5. Conclusion and discussion

In the preceding three sections we have analysed the structure of the perturbation expansions of the two-dimensional ANNNI and 4ASC models about points at which these models reduce to simple Ising models. The main conclusions emerging from this analysis are the following.

(i) For small J_2, the ANNNI model continues to exhibit an Ising-like transition. The Müller-Hartmann–Zittartz result (2.19) is however in error at first order in $\kappa = J_2/J_1$. The principal formulae are (2.20) and (2.17).

(ii) For small J_1, i.e. large $\kappa = J_2/J_1$, the perturbation expansion around $J_1 = 0$ is considerably more complicated (expression (3.43)). Indeed, the coefficient of the second-order term is *more* singular than the unperturbed free energy. This suggests that the perturbation is valid only for fixed $T > T_c(J_1)$ and breaks down as T approaches $T_c(J_1)$. On the basis of the singularity structure of the perturbation expansion to second order in $w_1 = \tanh \beta J_1$, we then *conjectured* a scaling form (3.44) for the free energy in the *uniform* limit $J_1 \to 0$, $T \to T_c$.

(iii) To second order in Δ, the perturbation expansion of the free energy of the 4ASC model is identical (under an appropriate correspondence of coupling constants (4.5)) to that found for the ANNNI model about $\kappa = \infty$ ($J_1 = 0$). This suggests that the 4ASC model for small Δ and the ANNNI model for large κ behave similarly. This is probably the most significant conclusion of the paper and one we now want to discuss in more detail.

The topology of the phase diagrams of the two-dimensional ANNNI and 4ASC models, that has emerged from recent work (for detailed references see § 1), is illustrated in figure 1. Our main interest is in the regions of large κ in the ANNNI model and of small Δ in the 4ASC model†.

The phase diagram for the ANNNI model, depicted in figure 1(*a*), is based primarily on the results of the analysis of extensive weak-coupling (low-temperature) and strong-coupling (high-temperature) expansions in $1/\lambda$ and λ respectively of the quantum Hamiltonian analogue (2.22) (Barber and Duxbury 1981a, b). As discussed in § 3, the results of this analysis for $\kappa < \frac{1}{2}$ agree extremely well with the boundary deduced from the expansion around $\kappa = 0$. For $\kappa \geq 1.1$, Barber and Duxbury (1981b) concluded that only a single transition occurred directly from the paramagnetic phase to the (2, 2) antiphase state; i.e. the incommensurate phase does not persist to $\kappa = \infty$. However, the accuracy to which the boundary could be located from both sides is much less than for $\kappa < \frac{1}{2}$. Thus the possibility of a thin 'tongue' of incommensurate phase extending to $\kappa = \infty$ cannot be completely excluded. Subsequent finite-lattice calculations (Barber and Duxbury 1981a, Duxbury and Barber 1981) also tend to favour a single transition but likewise would have difficulty resolving a very thin strip.

Evidence that the incommensurate phase in the ANNNI model *does extend to* $\kappa = \infty$ comes from Monte Carlo calculations (Selke 1981) of (1.1) on finite lattices. At least for $\kappa < 4$ (the extent of the simulations), Selke found evidence (specific heat peaks, non-zero wavevector modulation of the ordered phase) for two transitions. However, this conclusion is also not equivocal since the two apparent transitions could conceivably coalesce for an infinite system.

Turning now to the 4ASC model, the situation is less satisfactory because of a lack of any quantitative data on the phase diagram. The diagram depicted in figure 1(*b*) is that suggested by Ostlund (1981) who argued that the incommensurate phase persisted to $\Delta = 0$. His argument is however qualitative and can be summarised as follows. Recall the behaviour of the p-state *symmetric* clock models. For $p > 4$, these are known to exhibit two transitions with the intermediate phase massless (José *et al* 1977, Elitzur *et al* 1979, Cardy 1980). The intermediate phase can be mapped (by renormalisation group arguments) onto the fixed line of the gaussian model, the two transitions then corresponding respectively to vortex fugacity and the p-state symmetry breaking field becoming relevant. Physically, the two transitions can be characterised (Einhorn *et al* 1980) as due to vortex unbinding (at $T = T_U$) and domain wall formation (at $T = T_L < T_U$).

In the four-state symmetric models, the two transitions coincide, the temperature corresponding to the gaussian model point at which the four-state symmetry breaking field and the vortex fugacity are simultaneously marginal (José *et al* 1977). Ostlund (1981) then argued that in the asymmetric models, the role of Δ is to separate the two transition mechanisms leading, even in the four-state model, to two transitions at distinct temperatures‡. That is, in essence Δ acts to effectively increase p. The weakness of this otherwise rather attractive argument lies in its tacit assumption that Δ itself is at worst marginal at the point $\Delta = 0$. The *relevance* of Δ as exhibited by our perturbative results suggests that the behaviour for $\Delta > 0$ could be significantly

† The 4ASC model is symmetric about $\Delta = \frac{1}{2}$ so our remarks apply equally to Δ near 1.

‡ I am grateful to Dr M Einhorn and Dr J Hirsch for a very illuminating discussion on this point.

different. Clearly, a quantitative investigation of the phase diagram of the 4ASC model would be of considerable interest.

One other point should be mentioned at this stage. It is conceivable that the difference between the conclusions of Barber and Duxbury (1981a, b) and of Selke (1981) concerning the ANNNI model is due to the Hamiltonian limit, i.e. the ANNNI model in the extremely anisotropic limit (2.21) behaves differently than when the anisotropy of the nearest-neighbour interaction is finite (the situation in Selke's Monte Carlo work). While there is no evidence that a Hamiltonian limit such as (2.21) is not innocuous, it is certainly the case that certain effects can be much smaller in the Hamiltonian version of a theory. For example, the extent of the massless phase in the Hamiltonian version of the symmetric five-state model is very small (Hamer and Barber 1981), whereas in the isotropic model a rather more extensive phase appears possible (Domany *et al* 1980). A similar effect could easily occur in the ANNNI model. At this stage, however, no firm conclusion on the precise details of the phase diagram of either the 4ASC or the ANNNI model can obviously be drawn.

Despite the rather unsatisfactory situation described in the previous paragraphs it is interesting at least to speculate on some of the other implications of a form such as (3.44) for the free energy of the ANNNI model near $\kappa=\infty$ and the 4ASC model near $\Delta=0$. The first concerns the possible non-universality apparent in (3.44). For this to be actual and not effective in the sense discussed in § 1, the scaling function $Q(z)$ of (3.44) would need to satisfy

$$Q(z)=Q_\infty+\mathrm{o}(1) \qquad \text{as } z\to\infty. \tag{5.1}$$

We know of no evidence from other methods to suggest that the phase boundary for large κ is truly non-universal. Indeed, the precise nature of the transitions is unclear, the quantum Hamiltonian series of Barber and Duxbury (1981a, b), for example, being too short and irregular to do more than locate the boundary. On the other hand, the order parameter in the antiphase state is two-dimensional,

$$\psi=\lim_{N\to\infty}\frac{1}{N}\Big\langle\sum_{(m,n)}\exp(\mathrm{i}q_m)s_{m,n}\Big\rangle \tag{5.2}$$

being a possible representation, where $q_m=2\pi(m-1)/4$. The appropriate Landau free energy, incorporating the relevant symmetries of (1.1), then has an expansion through fourth order of the form†

$$F=r|\psi|^4+u|\psi|^4-v(\psi\psi^*+\psi^*\psi). \tag{5.3}$$

This is of the same form as the Landau free energy of the Ashkin–Teller or eight-vertex models for which non-universality is known to occur. The relationship between the ANNNI model and the eight-vertex model has also been discussed by Rujan (1981), who showed that (1.1) could be mapped onto an eight-vertex model with direct and staggered fields. While this mapping does not necessarily imply non-universal behaviour, the possibility should clearly be kept in mind, particularly if the phase diagram is as shown in figure 1(a) with a single phase boundary for large κ.

Finally, we note that if the incommensurate phase does indeed persist to $\kappa=\infty$ in the ANNNI model or to $\Delta=0$ in the 4ASC model, several conjectures are available for the nature of the transitions. The upper transition from paramagnetic to incommensurate

† For a review of the classification of phase transition by symmetry arguments based on Landau free energy expansions see Barber (1980).

is expected (Garel and Pfeuty 1976) to be in the same universality class as the $d=2$ planar rotor model and thus to exhibit a Kosterlitz–Thouless transition. Evidence for this type of behaviour is apparent in the Monte Carlo simulations (Selke and Fisher 1980, Selke 1981) and more weakly in the quantum Hamiltonian data (Duxbury and Barber 1981). Such behaviour is also expected in the 4ASC model (Ostlund 1981, Cardy 1981).

At the lower transition (incommensurate to commensurate) much less is known. From the incommensurate side, a simple approximation—the 'free-fermion' approximation—predicts a square root singularity in the specific heat (Villain and Bak 1981, Rujan 1981). On the other side, this approximation suggests that the specific heat is finite. However, the free-fermion approximation is not expected to describe the commensurate phase particularly well and the true behaviour is an open question.

These various possibilities can obviously be incorporated into an appropriate form for the function $Q(z)$ in (3.44) at large z. However, in the absence of more substantial grounds for the validity of (3.44) this is rather a speculative exercise.

Acknowledgments

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Appendix 1

In this appendix, we outline the analysis of the first two orders of the expansion (2.23) for λ near $\lambda_c = 1$. The unperturbed ground state energy

$$E_0^0(\lambda) = -\frac{1}{\pi}\int_0^\pi (1+\lambda^2+2\lambda\cos\theta)^{1/2}\,\mathrm{d}\theta \tag{A1.1}$$

reduces easily (Pfeuty 1970) to the elliptic integral of the second kind,

$$E(k) = \int_0^{\pi/2} (1-k^2\sin^2\theta)^{1/2}\,\mathrm{d}\theta. \tag{A1.2}$$

Explicitly we have

$$E_0^{(0)}(\lambda) = -(2/\pi)(1+\lambda)E(k), \tag{A1.3}$$

where

$$k^2 = 4\lambda/(1+\lambda)^2. \tag{A1.4}$$

Turning to the second-neighbour ground state correlation $\langle\sigma_i^z\sigma_{i+2}^z\rangle_0$ given by (2.25)–(2.27), we find that the three integrals $L(n)$, $n=0,1,2$, required can be expressed in terms of $E(k)$ and the elliptic integral of the first kind

$$K(k) = \int_0^{\pi/2} \frac{\mathrm{d}\theta}{(1-k^2\sin^2\theta)^{1/2}}. \tag{A1.5}$$

Some straightforward but tedious algebra then gives

$$\langle\sigma_i^z\sigma_{i+2}^z\rangle_0 = [3\pi^2\lambda^2(1+\lambda)^2]^{-1}[(1+\lambda)^4(5-\lambda^2)E^2(k)+(1-\lambda^2)^3K^2(k) -2(1+\lambda)^2(1-\lambda^2)(3+\lambda^2)E(k)K(k)]. \tag{A1.6}$$

The asymptotic expansions (2.28) and (2.29) then follow from (A1.3) and (A1.6) via the expansions (Byrd and Friedman 1971)

$$E(k) = 1+\tfrac{1}{2}(k')^2[\ln(4/k')-\tfrac{1}{2}]+O(k'^4\ln k'), \tag{A1.7}$$

$$K(k) = \ln(4/k')+\tfrac{1}{4}(k')^2[\ln(4/k')-1]+O(k'^4\ln k'), \tag{A1.8}$$

where

$$k' = (1-k^2)^{1/2} = (1-\lambda)/(1+\lambda). \tag{A1.9}$$

Appendix 2

In this appendix, we expand the function (see (3.40))

$$G(z) = \int_z^\infty F(\rho)\frac{d}{d\rho}(\rho F'(\rho))\,d\rho \tag{A2.1}$$

for small z. The function $F(\rho)$ appearing in the integrand is the scaling function of the pair-correlation function defined in (3.32) of the anisotropic nearest-neighbour Ising model with interactions J_0 and J_2. We shall require the following properties of $F(\rho)$ (Wu *et al* 1976):

$$F(\rho) = O(e^{-\rho}), \qquad \rho\to\infty, \tag{A2.2}$$

$$F(\rho) = F_0\rho^{-1/4}\,e^{-\rho/2}[1+\tfrac{1}{2}\rho\ln\rho+\tfrac{1}{2}b\rho+O(\rho^2\ln\rho)], \qquad \rho\to 0, \tag{A2.3}$$

where

$$F_0 = (\sinh 2\beta_c J_0+\sinh 2\beta_c J_2)^{1/8}\,e^{1/4}2^{1/2}C_G^{-3}, \tag{A2.4}$$

with β_c determined by (3.8) and

$$C_G = 1.282247\ldots \qquad \text{(Glaisher's constant)} \tag{A2.5}$$

and

$$b = C_E - 3\ln 2+1 = -0.50226\ldots, \tag{A2.6}$$

with

$$C_E = 0.577216\ldots \qquad \text{(Euler's constant)}. \tag{A2.7}$$

Integrating (A2.1) by parts and using (A2.2) gives

$$G(z) = -zF(z)F'(z)-\hat{G}(z), \tag{A2.8}$$

with

$$\hat{G}(z) = \int_z^\infty \rho[F'(\rho)]^2\,d\rho. \tag{A2.9}$$

To expand $\hat{G}(z)$ for small z, we write it as an inverse Mellin transform:

$$\hat{G}(z)=\frac{1}{2\pi \mathrm{i}}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} M(p)z^{-p}\,\mathrm{d}p \tag{A2.10}$$

with

$$M(p)=\int_0^\infty z^{p-1}\hat{G}(z)\mathrm{d}z=-\frac{1}{p}\int_0^\infty z^p\hat{G}'(z)\,\mathrm{d}z, \tag{A2.11}$$

provided $\mathrm{Re}\, p>\frac{1}{2}$ which fixes the contour in (A2.10).

Substituting (A2.9), we then have

$$M(p)=\frac{1}{p}\int_0^\infty z^{p+1}[F'(p)]^2\,\mathrm{d}z. \tag{A2.12}$$

For small z, the integrand in view of (A2.3) behaves as $z^{p+1-5/2}$ so that $M(p)$ is analytic for $\mathrm{Re}\, p>\frac{1}{2}$.

The required expansion of $\hat{G}(z)$ now follows from (A2.12), successive terms of *increasing* order in z following the sequence of singularities of $M(p)$ for $\mathrm{Re}\, p\leq\frac{1}{2}$. To determine these, we write

$$[F'(\rho)]^2=\tfrac{1}{16}F_0^2\,\mathrm{e}^{-\rho}\rho^{-5/2}+w(\rho) \tag{A2.13}$$

where, as $\rho\to 0$,

$$w(\rho)=-\tfrac{3}{16}F_0^2\,\mathrm{e}^{-\rho}\rho^{-3/2}[\ln\rho+b-\tfrac{3}{4}\rho\ln^2\rho+\mathrm{O}(\rho\ln\rho)]. \tag{A2.14}$$

Hence

$$M(p)=\frac{1}{16p}F_0^2\Gamma(p-\tfrac{1}{2})+\frac{1}{p}\int_0^\infty z^{p+1}w(z)\,\mathrm{d}z, \tag{A2.15}$$

where $\Gamma(q)$ is the gamma function. Substituting (A2.14) in the integral in (A2.15) gives

$$\int_0^\infty z^{p+1}w(z)=-\tfrac{3}{16}F_0^2[\Gamma'(p+\tfrac{1}{2})+b\Gamma(p+\tfrac{1}{2})-\tfrac{3}{4}\Gamma''(p+\tfrac{3}{2})]+R(p), \tag{A2.16}$$

where $R(p)$ is analytic for $\mathrm{Re}\, p>-\frac{3}{2}$ and has a double pole at $p=-\frac{3}{2}$. Hence $R(p)$ gives a contribution to $\hat{G}(z)$ of $\mathrm{O}(z^{3/2}\ln z)$ which is of higher order than we shall require. The required terms follow from the singularities of $M(p)$ in $-\frac{3}{2}\leq p\leq\frac{1}{2}$, which are revealed by the expression

$$M(p)=\frac{1}{16p}F_0^2[\Gamma(p-\tfrac{1}{2})-3\Gamma'(p+\tfrac{1}{2})-3b\Gamma(p+\tfrac{1}{2})+(\tfrac{9}{4})\Gamma''(p+\tfrac{3}{2})]+R(p)/p, \tag{A2.17}$$

together with the known behaviour (Whittaker and Watson 1965) of the gamma function as $q\to -r$, $r=0,1,2,\ldots$:

$$\Gamma(q)=\frac{(-)^r}{(q+r)r!}+\mathrm{O}(1): \tag{A2.18}$$

$$\Gamma'(q)=\frac{(-)^{r+1}}{(q+r)^2r!}+\frac{(-)^r\psi(r+1)}{(q+r)r!}+\mathrm{O}(1), \tag{A2.19}$$

$$\Gamma''(q)=\frac{2(-)^r}{(q+r)^3r!}+\mathrm{O}((q+r)^{-2}), \tag{A2.20}$$

where in (A2.19) $\psi(q) = \mathrm{d}\ln\Gamma(q)/\mathrm{d}q$. These results give the residues of all the required poles of $M(p)$ in $-\frac{3}{2} \leq p \leq \frac{1}{2}$, except that at $p=0$. This is most easily determined by returning to (A2.15), which yields

$$Q_0 = \lim_{p\to 0} pM(p) = -F_0^2\sqrt{\pi}/8 + \int_0^\infty zw(z)\,\mathrm{d}z, \tag{A2.21}$$

the convergence of the integral being assured by (A2.2) and (A2.14).

A straightforward asymptotic analysis now gives

$$\hat{G}(z) = Q_0 + (F_0^2 z^{-1/2}/8)[1 + 3z\ln z + (3\psi(1) + 3b - 5)z - \tfrac{3}{4}z^2(\ln z)^2 + \mathrm{O}(z^2\ln z)] \tag{A2.22}$$

where $\psi(1) = -C_{\mathrm{E}}$. Combining this with the expansion of $F(z)F'(z)$ that follows from (A2.3) finally yields (3.41) where the coefficients are given explicitly by

$$g_0 = F_0^2/8 = (\sinh 2\beta_c J_0 + \sinh 2\beta_c J_2)^{1/4}\,\mathrm{e}^{1/2}C_{\mathrm{G}}^{-6}/4, \tag{A2.23}$$

$$\hat{Q}_0 = 8Q_0/F_0^2, \tag{A2.24}$$

$$\gamma = -3\ln 2 + 2(1 + C_{\mathrm{E}})/5. \tag{A2.25}$$

Appendix 3. The ANNNI model as a four-state model

For completeness, we formulate, in this appendix, the ANNNI model as a four-state model. To do so consider the Hamiltonian (1.1) and define

$$\boldsymbol{S}_{k,l} = (s_{2k,l}, s_{2k+1,l}) = (S_{k,l}^{(1)}, S_{k,l}^{(2)}). \tag{A3.1}$$

Then we can write (1.1) as

$$H = \sum_{(k,l)} V_1(\boldsymbol{S}_{k,l}) + V_2'(\boldsymbol{S}_{k,l}, \boldsymbol{S}_{k,l+1}) + V_2(\boldsymbol{S}_{k,l}, \boldsymbol{S}_{k+1,l}), \tag{A3.2}$$

where the sum is over the sites of a square lattice and

$$V_1(\boldsymbol{S}) = -J_1 S^{(1)}S^{(2)}, \tag{A3.3}$$

$$V_2'(\boldsymbol{S}, \boldsymbol{S}') = -J_0\boldsymbol{S}\cdot\boldsymbol{S}', \tag{A3.4}$$

$$V_2(\boldsymbol{S}, \boldsymbol{S}') = J_2\boldsymbol{S}\cdot\boldsymbol{S}' - J_1 S^{(2)}S^{(1)}. \tag{A3.5}$$

The new variables $\boldsymbol{S} = (S^{(1)}, S^{(2)})$ are obviously four-state variables. The similarity to the 4ASC model is revealed if we introduce 'angle' variables

$$\theta = 0, \pi/2, \pi, 3\pi/2 \tag{A3.6}$$

by the relations

$$S^{(1)} = \cos\theta - \sin\theta = \sqrt{2}\cos(\theta + \pi/4), \tag{A3.7a}$$

$$S^{(2)} = \cos\theta + \sin\theta = \sqrt{2}\sin(\theta + \pi/4). \tag{A3.7b}$$

Hence we obtain

$$V_1(\boldsymbol{S}) = -J_1\cos 2\theta, \tag{A3.8}$$

$$V_2'(\boldsymbol{S}, \boldsymbol{S}') = -2J_0\cos(\theta - \theta'), \tag{A3.9}$$

$$V_2(\boldsymbol{S}, \boldsymbol{S}') = 2J_2\cos(\theta - \theta') - J_1\cos(\theta + \theta') - J_1\sin(\theta - \theta'). \tag{A3.10}$$

The expression for V_2 can be further simplified by combining the first and last term to give

$$V_2(\boldsymbol{S}, \boldsymbol{S}') = -J_1 \cos(\theta + \theta') + J_1 R \cos(\theta - \theta' + \Delta) \tag{A3.11}$$

with

$$R = (1 + 4J_2^2/J_1^2)^{1/2} \tag{A3.12}$$

and

$$\Delta = \tan^{-1}(J_1/2J_2), \tag{A3.13}$$

the arc tangent to be taken in the first quadrant. Substituting (A3.8), (A3.9) and (A3.11) into (A3.2) gives the required representation of the ANNNI model as a four-state clock model, namely

$$H = -\sum_{(k,l)} [J_1 \cos 2\theta_{k,l} + 2J_0 \cos(\theta_{k,l} - \theta_{k,l+1}) + J_1 \cos(\theta_{k,l} + \theta_{k+1,l}) - RJ_1 \cos(\theta_{k,l} - \theta_{k+1,l} + \Delta)] \tag{A3.14}$$

with $\theta = 2\pi n_i/4$, $n_i = 0, 1, 2, 3$. The similarity, but not equivalence, to the 4ASC model as defined in (1.2) is evident.

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