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Hamiltonian studies of the two-dimensional axial next-nearest neighbour Ising (ANNNI) model: II. Finite-lattice mass gap calculations

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Abstract. The quantum Hamiltonian analogue of the two-dimensional ANNNI model is investigated by finite-lattice mass gap methods. By using lattice sizes capable of simulating systems of varying modulation, we are able to show the existence of a modulated phase between the paramagnetic and $\langle 2, 2\rangle$ antiphase regions. The modulation on the incommensurate to paramagnetic boundary is shown to vary and this variation is calculated as a function of the anisotropy. In addition we find evidence for an XY-like transition from the incommensurate to the paramagnetic phase and perhaps a non-universal transition from the paramagnetic phase to the antiphase.

1. Introduction

This paper is the second in a series devoted to a study of the spin Hamiltonian

$$H = -\sum \sigma_m^x - \lambda \sum (\sigma_m^z\sigma_{m+1}^z - \kappa\sigma_m^z\sigma_{m+2}^z) \tag{1.1}$$

where σ_m^x, σ_m^z are Pauli spin matrices defined at the sites of a one-dimensional chain and λ and κ are positive. This Hamiltonian is of interest because it is the quantum Hamiltonian analogue (Barber and Duxbury 1981, Rujan 1981) of the two-dimensional axial next-nearest neighbour Ising (ANNNI) model. This model is currently receiving considerable attention as one of the simplest systems to exhibit an incommensurate/commensurate phase transition (Hornreich *et al* 1979, Selke and Fisher 1980, Selke 1981, Villain and Bak 1981, Rujan 1981, Williams *et al* 1981, Barber and Duxbury 1981, 1982, references therein). It is also of direct relevance to transitions in lipid bilayers (Pearce and Scott 1982).

The first paper in this series (Barber and Duxbury 1982, hereafter referred to as I) introduced the Hamiltonian (1.1), reviewed the known analytic results relevant to its ground-state phase structure and, most significantly, developed and analysed various systematic weak-coupling (in $1/\lambda$) and strong-coupling (in λ) perturbation series. A summary of and comparison with other work on the ANNNI model was also given. We refer to I for a detailed introduction to the literature.

In this paper we study (1.1) using finite-lattice mass gap data in a manner used successfully on several quantum Hamiltonians (Hamer and Barber 1980, 1981a, b, c,

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Hamer 1981, Roomany *et al* 1980, Roomany and Wyld 1980, Barber and Richardson 1981). Some finite-lattice calculations for (1.1) have already been reported (Williams *et al* 1981). However, these calculations were performed only on chains of up to eight sites. This lattice size, as we shall see, is insufficient to locate the incommensurate–paramagnetic phase boundary or to probe the nature of the incommensurate phase.

This paper is arranged as follows. In § 2 we outline our method of calculation and introduce the relevant β-function approximants (Roomany and Wyld 1980) that form the basis of our analysis. Our detailed results are presented in § 3, and the paper closes with an overall summary in § 4. A preliminary report on some of this work has already appeared (Barber and Duxbury 1981).

2. Method of calculation

We follow the calculational scheme pioneered by Hamer and Barber (1980, 1981b, c). We break the Hamiltonian (1.1) into the form

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

where (rotating in spin space and adding a trivial constant)

$$H_0 = \sum_{m=1}^{M} (1 - \sigma_m^z) \tag{2.2}$$

and

$$V = -\sum_{m=1}^{M} (\sigma_m^x \sigma_{m+1}^x - \kappa \sigma_{m+1}^x - \kappa \sigma_m^x \sigma_{m+2}^x). \tag{2.3}$$

Here M is the number of sites in the chain and we apply periodic boundary conditions so that $\sigma_m^x = \sigma_{m+M}^x$. The eigenstates of H_0 are now used to form a matrix representation of H, which is then diagonalised. Our interest will focus on the two lowest-lying levels and hence the mass gap.

The ground state ϕ_0 of H_0 is non-degenerate and such that $\sigma_m^z \phi_0 = \phi_0$ for all $m = 1, 2, \ldots, M$. This state is manifestly translationally invariant. Excited states are obtained from ϕ_0 by overturning sets of spins. In particular, the first excited state consists of a single overturned spin. This energy level is M-fold degenerate, the states being specified by

$$\phi_{1,m} = \sigma_m^x \phi_0 \qquad m = 1, 2, \ldots, M. \tag{2.4}$$

In view of the translational invariance of H, we form the linear combinations

$$\phi_{1,k} = M^{-1/2} \sum_{m=1}^{M} \exp 2\pi \mathrm{i} km/M) \phi_{1,m} \qquad k = 0, 1, 2, \ldots, M-1. \tag{2.5}$$

These states diagonalise V breaking the degeneracy of the first excited state of H_0 and leading to the expression

$$E_1(k) = 2 - 2\lambda\phi(2\pi k/M) + \mathrm{O}(\lambda^2) \qquad k = 0, 1, \ldots, M-1 \tag{2.6}$$

where

$$\phi(\theta) = \cos\theta - \kappa \cos 2\theta \tag{2.7}$$

for the resulting set of discrete levels. In the limit $M \to \infty$, this set forms a continuous band (Rujan 1981, Barber and Duxbury 1982). The mass gap is determined by the lowest edge of this band which is given by (2.6) with

$$q = 2\pi k/M = \begin{cases} 0 & \kappa < \frac{1}{4} \\ \cos^{-1}(1/4\kappa) & \kappa > \frac{1}{4}. \end{cases} \tag{2.8}$$

These first-order perturbation theory results imply that the first excited state of H no longer lies in the $k = 0$ sector for $\kappa > \frac{1}{4}$. While we shall see that this conclusion is, in fact, not true for $\kappa < \frac{1}{2}$, it does indicate that we cannot restrict attention in our finite-lattice work to the $k = 0$ sector. This necessitates some changes in the calculational scheme developed by Hamer and Barber (1980, 1981b).

We observe that the perturbation V is translationally invariant and flips two spins. Thus we can divide the state space of H_0 up into sectors labelled by k and 'parity', where the parity of a state is even (odd) if that state is obtained from ϕ_0 by overturning an even (odd) number of spins. On a finite lattice with periodic boundary conditions, the ground state of H lies in the even-parity $k = 0$ sector, while the first excited state lies in an odd-parity sector with a value of k that will turn out to depend upon κ and λ. However, there are no matrix elements between different k sectors. Thus we can use the Lanczos recursion method (Hamer and Barber 1981b, Roomany *et al* 1980) at specified κ and starting from the states $\phi_{1,k}$ to find the lowest eigenvalue in each odd-parity k sector. The lowest-lying excited state of H and hence the mass gap can then be determined by inspection. The fact that the resulting matrix representation of H is Hermitian rather than real symmetric causes no problems in the implementation of the Lanczos procedure.

The decomposition of the state space of H into sectors labelled by k is not only of computational significance. It also facilitates the identification (from finite-lattice data) of transitions to the modulated phase. On an infinite lattice, a transition to a modulated phase is marked by a divergence in the structure factor (or wavevector-dependent susceptibility) $\chi(q)$ for some $q \neq 0$ (see e.g. Redner and Stanley 1977, Hornreich *et al* 1979, Selke 1981). A quantum Hamiltonian analogue of $\chi(q)$ can be defined as follows.

Augment (2.1) with a wavevector-dependent field and consider

$$H(q) = H + h\sqrt{M}S_q \tag{2.9}$$

where

$$S_q = \frac{1}{\sqrt{M}} \sum_{m=1}^{M} \exp(2\pi \mathrm{i} q m)\sigma_m^x \tag{2.10}$$

with $q = k/M$, $k = 0, 1, 2, \ldots, M-1$. The wavevector-dependent susceptibility $\chi(q)$ is then defined by

$$\chi(q) = \lim_{M\to\infty} -M^{-1} \frac{\partial^2 E(q)}{\partial h^2}\bigg|_{h=0} \tag{2.11}$$

where $E(q) = E(h, \lambda, q)$ is the ground-state energy of (2.9). Applying second-order perturbation theory to (2.9) gives

$$\chi(q) = \lim_{M\to\infty} -\frac{1}{M} \sum_{\alpha} \frac{|\langle 0|S_q|\alpha\rangle|^2}{E_0 - E_\alpha} \tag{2.12}$$

where E_0 is the ground-state energy of H and the sum is over all excited states $|\alpha\rangle$

of H. However, not all states contribute to the sum because of selection rules. To determine these recall that the ground state $|0\rangle$ is in the even-parity, $k = q = 0$ sector. The operator S_q flips a single spin and hence the state $S_q|0\rangle$ lies in the odd-parity, $k = qM$ sector. Thus the sum in (2.12) is only over those states in this sector. A divergence in $\chi(q)$ is heralded by the vanishing of a denominator in (2.12), i.e. a vanishing of the mass gap between E_0 and the lowest-lying excited state in the $k = qM$ sector.

On a finite lattice $\chi(q)$ is not divergent, but criticality should be reflected in a scaling as M^{-1} of the relevant mass gap (Hamer and Barber 1980). This will be our criterion for detecting a transition to a modulated phase.

In the limit $M \to \infty$, q is a continuous variable. For example, in the free-fermion approximation (Villain and Bak 1981, Rujan 1981) q is related to the wall density and changes continuously from $q = 0$ to $q = \frac{1}{4}$ on passage through the incommensurate phase from the ferromagnetic phase to the antiphase. On the other hand, on a finite chain of M sites q is restricted to the discrete values

$$q = k/M \qquad k = 0, 1, 2, \ldots, [M/2] \tag{2.13}$$

where $[x]$ is the largest integer not exceeding x. Moreover, the extrapolation to the infinite limit must be done at *fixed* q if we wish to detect a transition to a phase with modulation $q = k/M$. Hence, we must restrict attention to the sequence of lattices of size $\{M_n = n/q;\ n = 1, 2, 3, \ldots\}$. This restriction severely reduces the amount of lattice data we have available and consequently the precision we can reach. In particular, the sophisticated extrapolation procedures developed by Hamer and Barber (1981c) cannot, for the most part, be applied with the data currently available.

Using the Lanczos procedure as described in the previous paragraphs we have obtained the lowest-lying eigenvalues for lattices up to $M = 18$. This data allows us to probe the existence of modulated phases with $q = 0, \frac{1}{4}, \frac{2}{9}, \frac{1}{5}, \frac{1}{6}, \frac{1}{7}$ and $\frac{1}{8}$. To locate possible transitions we have used finite-size scaling theory (Fisher and Barber 1972, Hamer and Barber 1980) and the Roomany–Wyld approximants (Roomany and Wyld 1980)

$$\beta^{\mathrm{RW}}(\kappa, \lambda) = \frac{1 + \ln(\Lambda_1/\Lambda_2)/\ln(M_2/M_1)}{\sqrt{(\partial \ln \Lambda_1/\partial\lambda)(\partial \ln \Lambda_2/\partial\lambda)}} \tag{2.14}$$

to the exact beta function of (1.1). Here, $\Lambda_i = \Lambda_i(\kappa, \lambda, M_i)$ is the mass gap on a lattice of size M_i, $i = 1, 2$. These are calculated as a function of λ at fixed κ and q $(= k_1/M_1 = k_2/M_2$ for appropriate k_1 and k_2 on the two lattices). Due to the loss of orthogonalisation in the Lanczos tridiagonalisation we were unable to find the required derivatives of Λ with respect to λ by the Feynman–Hellmann theorem and evaluated them instead by direct numerical differentiation.

The approximants (2.14) have proved to be a very successful way of inferring the existence and nature of phase transitions in an infinite system from finite-lattice data (see e.g. Roomany and Wyld 1980, 1981, Hamer and Barber 1981c, Nightingale and Schick 1982). Let us recall their salient features. Unlike the exact β function of the finite system, which cannot vanish by virtue of the absence of any phase transition, the Roomany–Wyld approximants can exhibit a physical zero. The condition for β^{RW} to vanish, namely

$$\Lambda_1(\lambda)/\Lambda_2(\lambda) = M_2/M_1, \tag{2.15}$$

is identical to the phenomenological renormalisation criterion for criticality (Nightingale 1976, Sneddon and Stinchcombe 1979, Hamer and Barber 1980, 1981a, b), which reflects the finite-size scaling,

$$\Lambda(\lambda_c, M) \sim M^{-1} \tag{2.16}$$

of the mass gap at criticality.

Two types of critical behaviour will be of interest to us here. The first type is a conventional second-order transition to an ordered phase, marked by an algebraic singularity in the mass gap of the infinite system

$$\Lambda(\lambda, M=\infty) \sim (\lambda_c - \lambda)^{\nu} \qquad \lambda \to \lambda_c \tag{2.17}$$

and a simple zero in the exact β function

$$\beta(\lambda, M=\infty) \sim \nu^{-1}(\lambda_c - \lambda) \qquad \lambda \to \lambda_c \tag{2.18}$$

where the slope of $\beta(\lambda)$ at λ_c is determined by ν. The Roomany–Wyld approximants are expected to similarly exhibit a simple zero, satisfying (2.15), and approximating the exact critical coupling λ_c. In addition, the slope of β^{RW} at the zero yields an estimate of ν via (2.18). These expectations have been confirmed in several models (see e.g. Roomany and Wyld 1980, Hamer and Barber 1981c).

The criterion (2.15) is however powerful enough to detect more complex critical behaviour, in particular a Kosterlitz/Thouless-like transition to a massless phase (Hamer and Barber 1980, 1981b, Roomany and Wyld 1980, Barber and Richardson 1981). In this case, the exact infinite-lattice mass gap behaves as $(a, \sigma > 0)$

$$\Lambda(\lambda, M=\infty) \sim \exp[-a(\lambda_c - \lambda)^{-\sigma}] \qquad \lambda \to \lambda_c^- \tag{2.19}$$

with $\Lambda = 0$ for $\lambda > \lambda_c$, while

$$\beta(\lambda, M=\infty) \sim A(\lambda_c - \lambda)^{1+\sigma} \qquad \lambda \to \lambda_c^-. \tag{2.20}$$

Similar behaviour is expected in β^{RW}; estimates of λ_c and σ following by fitting the numerical results to (2.20) (Roomany and Wyld 1980). The possibility of this type of critical behaviour is of interest here because of the argument (Garel and Pfeuty 1976) that a transition from paramagnetism to an incommensurately ordered phase should be the same universality class as the two-dimensional XY model, for which $\sigma = \frac{1}{2}$ (Kosterlitz 1974).

3. Results

While matrix elements of V between states in different k sectors vanish, this does not imply (as stated by Rujan 1981) that the first-order perturbation expansion (2.6) for the first excited state determines the appropriate k sector for all λ. Level crossings may still occur and as shown in figure 1 definitely do occur as λ is varied at fixed κ. This figure shows the lowest-lying excited states (relative to the ground-state energy) on a 12-site chain with $\kappa = 0.40$. The states labelled $k = 1, 2$ are doubly degenerate (corresponding to $k = 11, 10$, respectively). For sufficiently small λ the $k = 2$ state is the lowest-lying state in accord with the first-order perturbation expansion (2.6). Two level crossings occur as λ increases and for $\lambda > 3.74$ the $k = 0$ state becomes the lowest-lying excited state thereby determining the mass gap which enters into the finite-size scaling analysis and, in particular, β^{RW} as defined by (2.14).

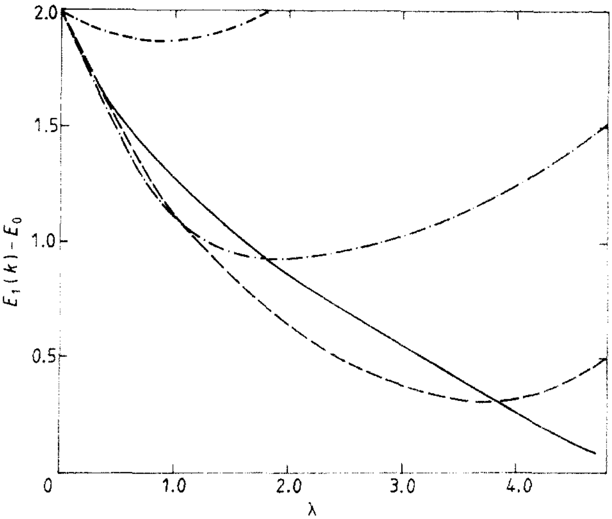

Figure 1. Lowest-lying energy levels (see text) in the odd-parity sector of $M = 12$ site chain for $\kappa = 0.40$. Levels shown are $k = 0$ (——), $k = 1, 11$ (- - - -), $k = 2, 10$ (- · - · - ·), $k = 3, 9$ (- - · - - · - - ·). Levels for other k lie above those shown.

The behaviour illustrated in figure 1 is typical of that found for all $\kappa < \frac{1}{2}$. For $\kappa < \frac{1}{4}$ the $k = 0$ state is the lowest-lying excited state for all λ. For $\frac{1}{4} < \kappa < \frac{1}{2}$, the first-order perturbation result (2.6) determines the lowest-lying k state (as expected) for small λ. At larger λ one or more level crossings occur with $k = 0$ ultimately becoming the true state and determining the critical behaviour.

The Roomany–Wyld approximants (2.14) to the β function following from the $k = 0$ mass gaps are shown in figures 2 and 3 for $\kappa = 0.225$ and $\kappa = 0.40$. A single,

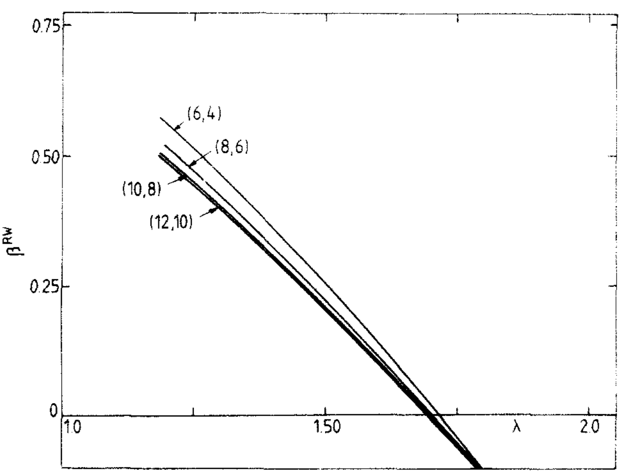

Figure 2. Roomany–Wyld approximants β^{RW} to the β function at $\kappa = 0.225$ formed from mass gap data for indicated lattice sizes.

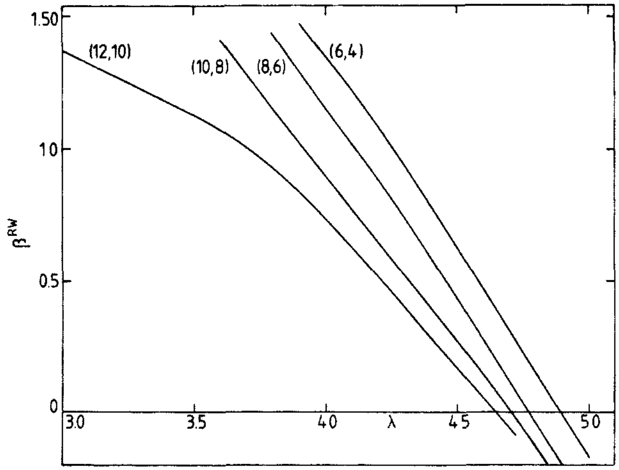

Figure 3. Roomany–Wyld approximants β^{RW} at $\kappa = 0.40$ formed from mass gap data for indicated lattices.

simple algebraic transition is clearly suggested. From the zeros of the approximants we estimate

$$\lambda_c(\kappa) = \begin{cases} 1.690 \pm 0.005 & \kappa = 0.225 \\ 4.60 \ \ \pm 0.05 & \kappa = 0.40 \end{cases} \tag{3.1}$$

while the slope at the zero gives the estimates

$$\nu = \begin{cases} 0.98 \pm 0.04 & \kappa = 0.225 \\ 0.95 \pm 0.10 & \kappa = 0.40. \end{cases} \tag{3.2}$$

These estimates of λ_c can be compared with those from *weak*-coupling series about $\lambda^{-1} = 0$ (Barber and Duxbury 1982), namely

$$\lambda_c(\kappa) = \begin{cases} 1.6938 \pm 0.0003 & \kappa = 0.225 \\ 4.627 \ \ \pm 0.002 & \kappa = 0.40. \end{cases} \tag{3.3}$$

The agreement between (3.1) and (3.3) is excellent and confirms the existence of a single Ising-like transition. Similar results are found for all $\kappa < \frac{1}{2}$.

For $\kappa > \frac{1}{2}$ the situation is more complicated, as was already evident from the perturbation series analyses reported in I. The advantage of the finite-lattice approach is that we can probe the modulated phase directly. In particular, we look for indications of a transition to a phase with modulation specified by q with $0 < q < \frac{1}{4}$. The $q = \frac{1}{4}$ mass gap data is found by using lattices of size $M = 4, 8, 12, 16$. The ground state, as always, is in the even-parity $k = 0$ sector and the appropriate first excited state lies in the odd-parity $k = M/4$ sector. To test for a transition to a phase with arbitrary modulation q, $0 < q < \frac{1}{4}$, we require lattices of size $M = n/q$, $n = 1, 2, \ldots$, for which the appropriate excited state lies in the $k = Mq$ sector.

Using the available lattice sizes, we construct an approximate critical curve by testing the criticality of finite-size systems modelling infinite systems with modulation $q = \frac{1}{8}, \frac{1}{7}, \frac{1}{6}, \frac{1}{5}, \frac{2}{9}$ and $\frac{1}{4}$. For most of these q values we only have one pair of lattice sizes to work with and hence we cannot claim to know the infinite lattice equivalent with precision. However, by determining the q sector of the first mass gap to scale, we believe a reasonable approximation to the true behaviour can be surmised. Figures 4 and 5 show scaled mass gap plots at $\kappa = 0.90$ and $\kappa = 1.25$, respectively. From these plots we conclude that at $\kappa = 0.90$, the $q = \frac{1}{5}$ mass gap is no longer critical while the $q = \frac{2}{9}$ still is. At $\kappa = 1.25$ we conclude that neither the $q = \frac{1}{5}$ nor the $q = \frac{2}{9}$ system is critical.

By repeating this type of analysis for various values of κ in the interval $\kappa > \frac{1}{2}$ we can generate the sequence of steps shown in figure 6 as an approximation to the critical q curve along the paramagnetic/incommensurate phase boundary. The infinite-lattice critical q curve can be expected to lie *beneath* the steps since, except at fortuitous values of κ, the transitions detected will be *inside* the incommensurate phase. A possible infinite-lattice extrapolation of our finite-lattice curve is shown by the full line in figure 6.

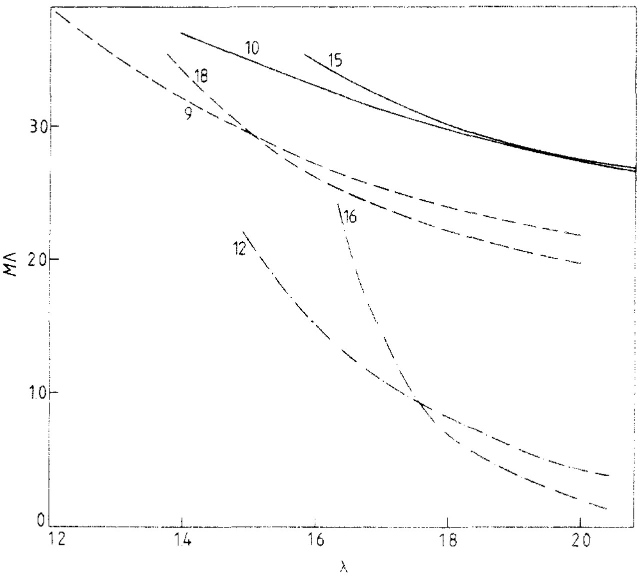

Figure 4. Scaled mass gaps for $q = \frac{1}{5}$ (——), $\frac{2}{9}$ (– – –), $\frac{1}{4}$ (– · – ·) at $\kappa = 0.90$.

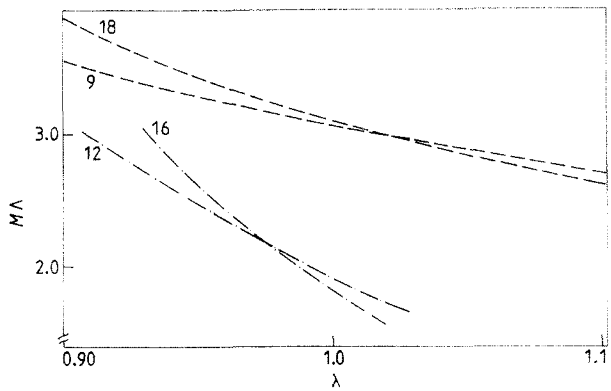

Figure 5. Scaled mass gaps for $q = \frac{2}{9}$ (– – – –), $\frac{1}{4}$ (– · – ·) at $\kappa = 1.25$.

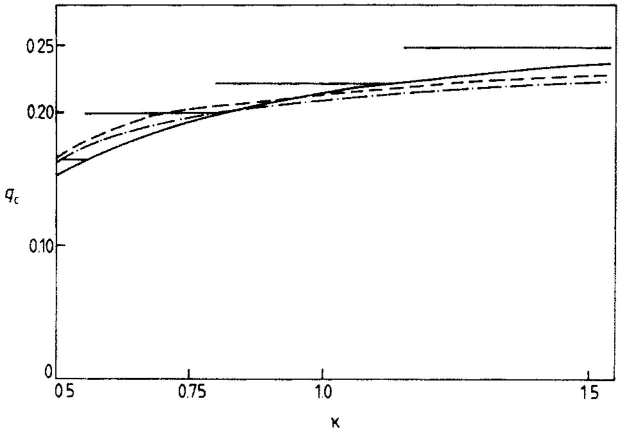

Figure 6. Variation of q_c as a function of κ. The estimate based on finite-lattice data is the step-wise function; with a possible infinite-lattice curve shown by the continuous line (——). The result for q_c from Monte Carlo calculations (Selke 1981) is shown by the broken line (- - - -), while the first-order result equation (2.8) is represented by the chain curve (– · – · –).

Selke (1981) has recently extended the Monte Carlo calculations of Selke and Fisher (1980) on the conventionally formulated ANNNI model. In particular, he studied $M\times 10$ systems with $176<M<352$ and located the various transitions from the specific heat peaks and their size dependence. In addition, he determined $q_c = q_c(\kappa)$ from the maximum in the structure factor $\chi(q)$. While care is required in comparing the results of the Monte Carlo calculations (performed on a (nearly) isotropic $d=2$ ANNNI model) and those of the quantum Hamiltonian (1.1) which involves a highly anisotropic limit (Barber and Duxbury 1982, Rujan 1981), it is interesting to superimpose Selke's results on ours as is shown also in figure 6. Selke's curve could possibly be the $M\to\infty$ limit of ours with one exception. Selke's curve (not shown) continues past $\kappa=\frac{1}{2}$ suggesting a Lifshitz point near $\kappa\sim 0.30$, where $q_c\to 0$. This is presumably a pseudocritical effect, and is inconsistent with recent arguments on the stability of incommensurate phases (Coopersmith *et al* 1981, Villain and Bak 1981) and our results.

The chain curve in figure 6 is the first-order perturbation result derived from equation (2.8) and it lies close to both our infinite-lattice conjecture and Selke's curve. We are unable to test for the presence of a Lifshitz point because the q value near this point could only be probed by very large lattices. The question of the existence of a Lifshitz point at finite κ is discussed further in the next section.

Figure 6 also suggests that at $\kappa=\frac{1}{2}$, q_c is discontinuous with

$$\lim_{\kappa\to\frac{1}{2}+} q_c(\kappa) = q_0 > 0 \tag{3.4}$$

where from figure 6, we estimate $q_0 \simeq 0.15$. While we have found no evidence of $q=\frac{1}{8}$ or $\frac{1}{7}$ ever becoming critical, it is extremely difficult to carry out detailed calculations for $\kappa\leqslant 0.55$. Thus a steep rise in q_c near $\kappa=\frac{1}{2}$ cannot be definitely excluded.

Figure 7 shows the Roomany–Wyld approximants at $\kappa=0.70$ constructed from mass gap data with q values of $g=\frac{1}{4}$ ($M=8, 12$), $q=\frac{1}{5}$ ($M=5, 10, 15$) and $q=\frac{1}{6}$ ($M=6, 12$). The approximant for $q=\frac{1}{6}$ clearly exhibits no sign of a transition, whereas

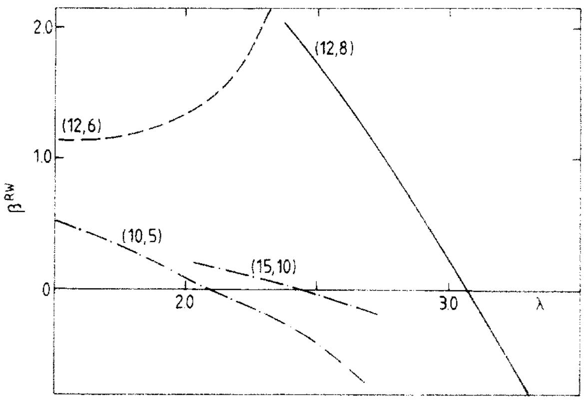

Figure 7. Roomany–Wyld approximants β^{RW} at $\kappa = 0.70$ formed from mass gap data for indicated lattices with $q = k/M = \frac{1}{4}$ (——), $\frac{1}{5}$ (– · – · –) and $\frac{1}{6}$ (– – – –).

the others exhibit zeros, with that of the $q = \frac{1}{5}$ approximants occurring at a smaller value of λ than the $q = \frac{1}{4}$ approximant. We believe (see further below) that the $q = \frac{1}{4}$ approximants locate the transition to the antiphase, while the $q = \frac{1}{5}$ approximants yield evidence of an incommensurately modulated phase.

The results presented in figure 7 thus confirm the picture that for $\kappa = 0.70$ the ANNNI Hamiltonian exhibits two transitions as λ varies; at λ_L to an incommensurate phase and then at λ_U to the antiphase. A reliable estimate of λ_L is clearly not available from our current data for two reasons. Firstly, the (10, 5) and (15, 10) approximants illustrated in figure 7 are not converged and secondly we have no data to test for an earlier transition to a phase with q between $\frac{1}{6}$ and $\frac{1}{5}$. Nevertheless, it is encourging that the zero of the (15, 10) approximant at $\lambda \simeq 2.45$ is very close to the paramagnetic/incommensurate boundary as located from disorder parameter series in I. This analysis gave $\lambda_L \simeq 2.5–2.6$.

The forms of the (10, 15) and (5, 10) approximants in figure 7 are also consistent with a Kosterlitz–Thouless transition, although any attempt to estimate the precise nature of the singularity is hardly warranted. Nevertheless, these approximants are very similar to low-order approximants obtained for the O(2) model (Roomany and Wyld 1980).

The antiphase boundary can be located by analysing the Roomany–Wyld approximant using $q = \frac{1}{4}$ mass gap data and lattices of size $M = 4, 8, 12, 16$. For $\kappa > 1.25$, these are the only approximants which are critical given our resolution. Typical results for $\kappa = 1.75$ are shown in figure 8 and are suggestive of a second-order transition. The precision of the estimates of the infinite-lattice results can be improved by the use of a simple three-term sequence extrapolation formula

$$S_\infty \simeq S_2 + \frac{(S_3 - S_2)(S_2 - S_1)}{2S_2 - S_3 - S_1} \tag{3.5}$$

based on Shanks's transform (Shanks 1955, Hamer and Barber 1981c). Here S_i are either of the estimates of λ_c and ν obtained from the $(4i+4, 4i)$ approximants. Using the data in figure 8 we estimate that

$$\lambda_c(\kappa = 1.75) = 0.64 \pm 0.02 \tag{3.6}$$

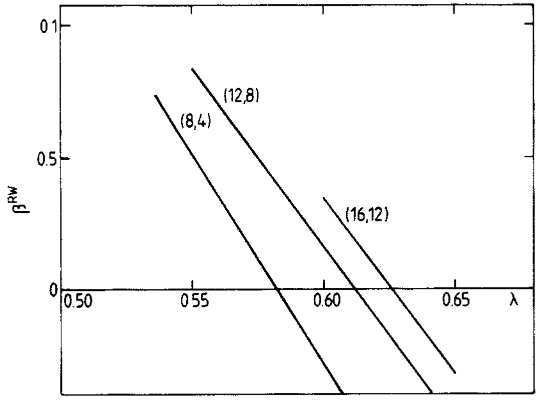

Figure 8. Roomany–Wyld approximants β^{RW} at $\kappa = 1.75$ formed from mass gap data for indicated lattices with $q = k/M = \frac{1}{4}$.

while

$$\nu(\kappa = 1.75) = 0.75 \pm 0.05. \tag{3.7}$$

The corresponding estimates of λ_c obtained in I were 0.67 ± 0.04 from the analysis of weak-coupling antiphase order parameter series and 0.63 ± 0.03 from the analysis of strong-coupling disorder parameter series. The agreement between these estimates and (3.6) is again remarkably good.

We have performed a similar analysis for several values of κ in the range $\kappa = 1.25$ to $\kappa = \infty$. The location of the phase boundary is consistently in excellent agreement with the series work of I. However, the estimate of the exponent ν is apparently a function of κ, as shown in figure 9. The significance of this is discussed in the next section.

For $\kappa = \infty$, or rather in the limit $\kappa \to \infty$, $\lambda \to 0$ with $\lambda' = \kappa\lambda$ fixed, (1.1) reduces to two uncoupled transverse Ising models (Barber and Duxbury 1981, Rujan 1981). Our finite-size analysis in this limit gives

$$\lambda_c' = 0.998 \pm 0.005 \tag{3.8}$$

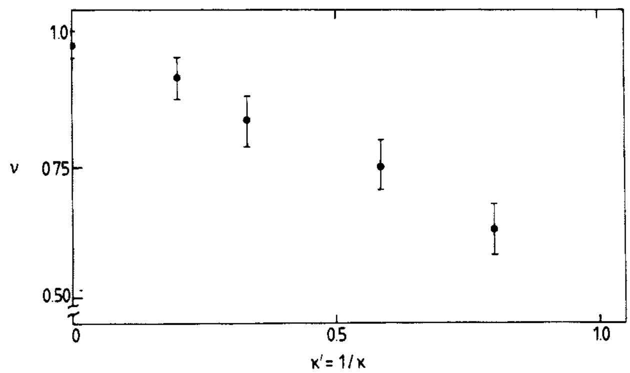

Figure 9. Variation of the estimates of the exponent ν as a function of $\kappa' = 1/\kappa$ along the antiphase boundary.

and

$$\nu = 0.98 \pm 0.05 \tag{3.9}$$

in excellent agreement with the expected behaviour.

4. Discussion

The finite-lattice calculations reported in this paper confirm and refine the conclusions drawn in I (Barber and Duxbury 1982) concerning the phase diagram of the ANNNI Hamiltonian (1.1).

For $\kappa < \frac{1}{2}$, this model exhibits a single Ising transition from paramagnetism to ferromagnetism. There is no incommensurate phase in agreement with recent arguments (Coopersmith *et al* 1981, Villain and Bak 1981, Peschel and Emery 1981). On the other hand, for $\kappa > \frac{1}{4}$, there is considerable structure in the excited-state band arising from level crossings between different k sectors. The effect this has on series expansions is not clear, but since the length of a series is closely related to lattice size (see I) extremely long series are probably required to extract the true critical behaviour. The anomalous results found in I for various series in the regime $0.35 < \kappa < 0.5$ are probably accounted for by this phenomenon.

These level crossings will also affect $\chi(q)$ as defined in (2.12), and in particular that $\check{\chi}(q)$ which is apparently divergent. This is presumably the explanation of the Lifshitz point 'found' near $\kappa \sim 0.35$ in Monte Carlo calculations (Selke and Fisher 1980, Selke 1981), series expansions (Redner, unpublished) and in our preliminary results (Barber and Duxbury 1981) on short series and smaller lattices.

For $0.5 < \kappa < \kappa_L \sim 1.1$, we confirm the conclusion of I that the transition from paramagnetism to the antiphase is via two transitions and an intermediate, probably massless, phase. The β-function approximants at the upper transition from paramagnetism are found to be indicative of a Kosterlitz/Thouless-like transition in accord with the prediction of Garel and Pfeuty (1976, see also Selke and Fisher 1980).

We are unable to locate the Lifshitz point due to our restriction to finite-size lattices. Near the Lifshitz point we expect the value of q_c to be tending to $\frac{1}{4}$, hence requiring large lattices to sample this behaviour. It does appear that if a Lifshitz point does exist at finite κ, the value of κ_L would be larger than the $\kappa_L \sim 1.1$ suggested in I.

Unlike the perturbation calculations of I, the finite-lattice calculations provide direct evidence that the intermediate phase is modulated. The modulation is characterised by a q vector between 0 and $\frac{1}{4}$; the values $q = 0$ and $q = \frac{1}{4}$ corresponding to the ferromagnetic and antiphases respectively. In principle, q should be a continuous function of both κ and λ (see e.g. Villain and Bak 1981). Unfortunately, one of the limitations of using chains small enough to allow the energy levels to be computed exactly is that q is restricted to a small set of discrete values. Consequently, we have only been able to determine the value $q_c = q_c(\kappa)$ of the modulation at the onset of the incommensurate phase with low resolution (recall figure 6), which, however, is similar to that found in Monte Carlo calculations (Selke 1981) for $\kappa > \frac{1}{2}$. At $\kappa = \frac{1}{2}$, there is an abrupt (possibly discontinuous) drop in q_c to zero.

In this context, it is important to note that to 'fit' a state with modulation between $q = 0$ and $q = \frac{1}{4}$ correctly and to have at least two lattices so that a sensible Roomany-Wyld approximant to the β function can be formed one needs lattices of size up to at least $M = 10$. Williams *et al* (1981) in their investigation of (1.1) via finite-lattice methods used lattices of only up to eight sites, which is insufficient to locate the incommensurate phase.

Finally, we turn to the antiphase boundary. This was located by scaling data from chains of M sites, with M an integral multiple of four. The resulting boundary was in excellent agreement with the series analyses of I. The estimates of the exponent ν are however κ dependent (recall figure 9) and suggest that the antiphase boundary above the Lifshitz point is non-universal. While this conclusion is in agreement with a suggestion made by one of us on the basis of perturbation expansions about $\kappa = \infty$ (Barber 1982), it may be spurious for two reasons. Firstly, if there is a thin tongue of incommensurate phase extending to $\kappa=\infty$, the use of $q=\frac{1}{4}$ lattice sizes would be incapable of modelling the incommensurate phase and hence incapable of making quantitative predictions about the nature of the incommensurate to antiphase transition. Secondly, if there is a Lifshitz point at finite κ, the non-universality observed may still be a simple crossover effect from one type of behaviour above the Lifshitz point to some other behaviour at or below the Lifshitz point. The clarification of these points clearly awaits conclusive evidence as to the location of the upper Lifshitz point.

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