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1989 J. Phys. A: Math. Gen. 22 5271

(http://iopscience.iop.org/0305-4470/22/24/015)

J. Phys. A: Math. Gen. **22** (1989) 5271-5279. Printed in the UK

Phase diagram for the spin-1 ANNNI model using the method of ring recurrence

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Received 7 June 1989

Abstract. The 2D spin-1 ANNNI model is studied using an iterative method, the method of ring recurrence. The phase diagram is obtained numerically using matrices of order 9. We find the phase diagram to be generally similar to that of the 2D spin-$\frac{1}{2}$ ANNNI model.

1. Introduction

The axial next-nearest-neighbour Ising (ANNNI) model (Elliott 1961) has been studied extensively in both two and three dimensions. It is one of the simplest statistical mechanical models to show complex modulated phases. A review of modulated structures in Ising models is given by Selke (1984). Recently Fuchs (1988) has used a modified transfer matrix method to analyse some properties of the two-dimensional ANNNI model. The 2D model is defined on the square lattice by nearest-neighbour couplings J along the x and z axes, and second-neighbour couplings J_2 along the z axis as well (figure 1). Some time ago we described the application of a new iterative scheme, the method of ring recurrence, to the 2D spin-$\frac{1}{2}$ ANNNI model (Saqi and McKenzie 1987). We showed that the method enabled the phase diagram to be obtained with minimal computational effort using low-order matrices. In the limiting case $J_2 = 0$, the method gives the critical point as $1.551 < \exp(J/kT) < 1.554$, which is in good

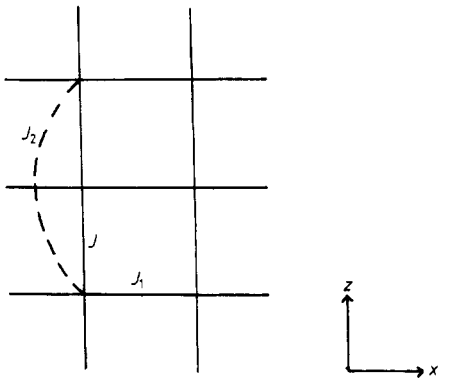

Figure 1. The two-dimensional ANNNI model. J and J_1 are ferromagnetic nearest-neighbour couplings. J_2 is the antiferramagnetic second-neighbour coupling along the z axis. We take $J = J_1$ in this study.

0305-4470/89/245271+09$02.50

agreement with the exact value (1.553). The method also allowed a direct calculation of the wavevector in the incommensurate phase. The phase diagram we obtained was in general agreement with other results (Villain and Bak 1981, Beale *et al* 1985). The phase diagram displays ferromagnetic (F), paramagnetic (P), incommensurate (I) and $++--$ (or $\langle 2 \rangle$) phases on varying the temperature and the ratio J_2/J. The $\langle 2 \rangle$ phase consists of two rows of 'up' spins, followed by two rows of 'down' spins along the z direction in the lattice. We observed the existence of the incommensurate phase for values of $-J_2/J_1$ less than 0.5. That is, as the temperature is lowered for $-J_2/J_1 \sim 0.49$ the phase changes from paramagnetic to incommensurate, back to paramagnetic and then ferromagnetic. Here we present the phase diagram of a 2D spin-1 ANNNI model. The method of ring recurrence enables us to obtain the phase boundaries using matrices of order 9 and we find that this 're-entrant' effect is much more apparent.

2. Methodology

We now give a description of the method of ring recurrence (McKenzie 1981, see also Saqi and McKenzie 1987). We consider first the general formalism, then the application to the spin-$\frac{1}{2}$ Ising model on the square lattice. We show how the ideas are readily extended to deal with competing interaction models—the spin-$\frac{1}{2}$ ANNNI model (Saqi and McKenzie 1987) and the spin-1 ANNNI model which is reported in this paper. We hope to explain the method in somewhat more detail than has previously been reported.

The method of ring recurrence provides a method of studying phase transitions on both Bethe and dimensional (Mckenzie 1981) lattices and is applicable to any model with a classical Hamiltonian. The method is formulated in terms of a discrete physical system (McKenzie 1981). This consists of a graph G, a set of localised states associated with each vertex $V(G)$ of the graph and a potential related to the edges $E(G)$ of the graph. The graph is the underlying space on which the system is embedded. The vertices of the graph are the physical entities (e.g. atoms). The edges indicate which atoms interact directly.

A graph is shown in figure 2. In the thermodynamic limit the effect of the edges become negligible, and the graph becomes the simple quadratic lattice. The potential U is

$$U = \beta H \sum_{X \in V(G)} \sigma_X + \beta J \sum_{[x,y] \in E(G)} \sigma_x \sigma_y + \beta J_2 \left(\sum_{A \subset G} \sigma_x \sigma_y \right). \tag{1}$$

The last term here indicates an interaction other than nearest neighbour. For example $A = \{x, y = x, y \in V(G), d_z(x, y) = 2\}$ where d_z is the graph metric in the z direction,

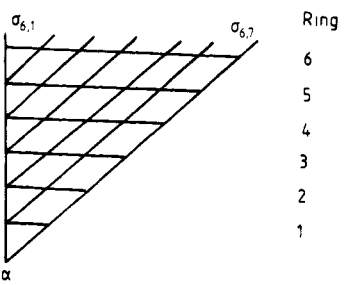

Figure 2. The 'wedge': α is the origin and rings are labelled as shown.

then we have the ANNNI model since we have included a second-neighbour coupling along the z axis.

Each of the horizontal lines in figure 2 is a 'ring' of the graph, X_s relative to the origin $\alpha \in V(G)$ where

$$X_s^\alpha = \{x: x \in V(G), d(x, \alpha) = s;\ s = 0, 1, 2, \ldots\}.$$

Clearly

$$\bigcup_{s \geqslant 0} X_s^\alpha = V(G).$$

The basic idea behind the method of ring recurrence is to build up the partition function in stages. Φ is the state space of the system. $\Phi = \Pi_{x \in V(G)} \phi_x$ where $\phi_x = \{1, -1\}$ for the spin-$\frac{1}{2}$ model or $\{+1, 0, -1\}$ for spin 1.

Let Ω_i be the state space associated with ring i. Then

$$\Omega_i = \prod_{x \in X_i} \phi_x \qquad \text{and} \qquad \Phi = \Pi \Omega_i$$

and let $\omega_i \in \Omega_i$.

Consider the interaction $J(\omega_i, \omega_j)$, $\omega_i \in \Omega_s$, $\omega_j \in \Omega_{s+1}$

$$J(\omega_i, \omega_j) = \sum_{x \in X_{s+1}} j_x + \sum_{e \in E_{s+1}} j_e + \sum_{e \in E_{s,s+1}} j_e$$

where

$$E_{s+1} = \{(x, y);\ x, y \in X_{s+1}\}$$

$$E_{s,s+1} = \{(x, y);\ x \in X_s,\ y \in X_{s+1}\}.$$

We see that there are contributions to $J(\omega_i, \omega_j)$ from vertices in ring $(s+1)$, edges in ring $(s+1)$ and the edges joining ring $(s+1)$ to ring (s). The partition function of a finite graph G_n for which $V(G_n) =$ can thus be written as

$$Z_{Gn} = \sum_{\omega \in \Omega_0} e^{J(\omega)} \left[\sum_{\omega_1 \in \Omega_1} e^{J(\omega, \omega_1)} \left[\sum_{\omega_2 \in \Omega_2} e^{J(\omega_1, \omega_2)} \cdots \left[\sum_{\omega_n \in \Omega_n} e^{J(\omega_{n-1}, \omega_n)} \right] \cdots \right] \right]. \tag{2}$$

We define normalised effective fields μ_s by

$$\mu_s(\omega_s) = \sum_{\omega_{s+1}} e^{J(\omega_s, \omega_{s+1})} \mu_{s+1}(\omega_{s+1}). \tag{3}$$

This defines recursion relations for the μ_s. The μ_s is a partial partition function for that portion of the graph located further than s rings from the origin. The recurrence relations give us an iterative scheme to study the problem of phase transitions. For an infinite graph we choose an arbitrary value of s and iteration gives $s-1$ and $s-2 \ldots$. The fixed point of the iteration represents what is happening 'deep inside' the lattice. For Bethe graphs the method is trivially exact (see for example McKenzie and Saqi 1986). For two-dimensional graphs (figure 2) the method of ring recurrence produces a matrix recursion and an approximation must be introduced to obtain a finite iterative scheme.

The effective fields μ_s for the graph in figure 2 can be expressed as a product of matrices. For the simple spin-$\frac{1}{2}$ Ising model

$$\mu_s = K_s(\sigma_{s,1}) A_s(\sigma_{s,1}) A_s(\sigma_{s,2}) \ldots A_s(\sigma_{s,s+1})$$

$$\mu_{s-1} = K_{s-1}(\sigma_{s-1,1}) A_{s-1}(\sigma_{s-1,1}) A_{s-1}(\sigma_{s-1,2}) \ldots A_{s-1}(\sigma_{s-1,s}).$$

The first subscript on the spin variable labels the ring and the second subscript labels the position of a spin along a ring. The $\boldsymbol{K}$ matrices are edge terms and are later neglected. There is a matrix recursion between the A_{s-1} and A_s.

For the spin-$\frac{1}{2}$ Ising model with nearest-neighbour interactions we have

$$\lambda A_{s-1}(\sigma) = \begin{pmatrix} x(\sigma)\,\mathrm{e}^{J}A_s(1) & x^{-1}(\sigma)\,\mathrm{e}^{-J}A_s(-1) \\ x(\sigma)\,\mathrm{e}^{-J}A_s(1) & x^{-1}(\sigma)\,\mathrm{e}^{J}A_s(-1) \end{pmatrix} \tag{4}$$

where

$$x(\sigma) = \exp(H + \sigma J)$$

$$x^{-1}(\sigma) = \exp(-H - \sigma J)$$

and λ is a norm.

The effective field is thus a product of matrices with a matrix associated with each vertex along the ring. There is a matrix recursion relating $A_{s-1}(\sigma)$ for ring $s-1$ to the equivalent matrix $A_s(\sigma)$ for ring s. Clearly, we do not have a sensible renormalisation scheme since at each step the matrices get bigger—$A_s(\sigma)$ is a (2×2), $A_{s-1}(\sigma)$ is a $(4\times 4)\ldots$, etc. Up to this stage, however, the formalism is exact. We note, however, the similarity between the matrix recursion and the recurrence relations of the Bethe graphs which are of the form

$$\mu_{s-1} = f(\mu_s).$$

To obtain a recurrence scheme the matrix recursion is reduced to a relation between scalars. The matrices $A_s(\sigma_{s,i})$ are diagonalised and contributions to the product $\Pi A_s(\sigma_{s,i})$, involving the largest eigenvalues only are retained.

Consider the product

$$\begin{aligned} \mu_s &= K_s(\sigma_{s,1})A_s(\sigma_{s,1})A_s(\sigma_{s,2})\ldots A_s(\sigma_{s,s+1})\mathbf{1} \\ &= K_s(\sigma_{s,1})\prod A_s(\sigma_{s,i})\cdot\mathbf{1}. \end{aligned} \tag{5}$$

Diagonalising the $A_s(\sigma_{s,i})$,

$$\mu_s = K_s(\sigma_{s,1})\prod T_s(\sigma_{s,i})M_s(\sigma_{s,i})T_s^{-1}(\sigma_{s,i})\mathbf{1} \tag{6}$$

where T_s is the matrix of eigenvectors and M_s is the matrix of eigenvalues. Equation (6) may be written as

$$\mu_s = K_s(\sigma_{s,1})T_s(\sigma_{s,1})\left(\prod_{i=1}^{s} M_s(\sigma_{s,i})T_s^{-1}(\sigma_{s,i})T_s(\sigma_{s,i+1})\right)M_s(\sigma_{s,s+1})T_s^{-1}(\sigma_{s,s+1}). \tag{7}$$

Define $T_s^{-1}(\sigma_{s,i})T_s(\sigma_{s,i+1})$ as the matrix with elements $a_{ij}(\sigma_{s,i}, \sigma_{s,i+1})$. Clearly for $\sigma_{s,i} = \sigma_{s,i+1}$ which corresponds to two adjacent spins in row s being in the same state, $a_{ii} = 1$. Neglect edge terms and consider the product

$$\mu_s = \prod_{i=1}^{s} M_s(\sigma_{s,i})T_s^{-1}(\sigma_{s,i})T_s(\sigma_{s,i+1}).$$

Neglecting all smaller eigenvalues leads immediately to

$$\mu_s \approx \prod_{i=1}^{s} \lambda_1(\sigma_{s,i}) \prod_{i=1}^{s} a_{11}(\sigma_{s,i}, \sigma_{s,i+1}). \tag{8}$$

We see that μ_s is the product of scalars:

$$\mu_s = \lambda(\sigma_{s,1})a_{11}(\sigma_{s,1}, \sigma_{s,2})\lambda_1(\sigma_{s,2})\ldots a_{11}(\sigma_{s,s-1}, \sigma_s)\lambda_1(\sigma_s).$$

We can thus associate a parameter $\lambda_1(\sigma_{s,i})$ with each vertex in ring s and a parameter $a_{11}(\sigma_{s,i}, \sigma_{s,i+1})$ with each edge within the ring.

The recursion relation (4), for the spin-$\frac{1}{2}$ Ising model thus becomes in this approximation

$$A_{s-1}(\sigma) = \begin{pmatrix} x(\sigma)\,\mathrm{e}^{J}\lambda_1(1) & x^{-1}(\sigma)\,\mathrm{e}^{-J}\lambda_1(-1)a_{11}(1,-1) \\ x(\sigma)\,\mathrm{e}^{-J}\lambda_1(1)a_{11}(-1,1) & x^{-1}(\sigma)\,\mathrm{e}^{J}\lambda_1(-1) \end{pmatrix}. \tag{9}$$

We describe the $a_{11}(\sigma_{s,i}, \sigma_{s,i+1})$ as the ring bond terms since they depend on the states of adjacent vertices in the same ring—ring s.

We introduce the matrix of ring bond terms, $\boldsymbol{B}$, with elements b_{ij} where

$$b_{ij} = a_{11}(i, j) \tag{10}$$

which refers to two adjacent vertices in a given ring that are in spin states i and j respectively. For the spin-$\frac{1}{2}$ Ising model, i and j take values $1(=+1)$ and $2(=-1)$ only. For the q-state Potts models i and j each takes values $1, 2, 3, \ldots, q$. Clearly from the definition of the ring bond terms, $b_{ii} = 1$.

The recursion relation is studied numerically by computing the matrices $A(\sigma)$ and their eigenvalues and eigenvectors for arbitary initial values of $\lambda_1(\sigma)$ and $a_{11}(\sigma_i, \sigma_{i+1})$. The critical point T_c is obtained from the behaviour of the fixed point μ^*. For $T > T_c$, $\mu^* = 1$, whilst for $T < T_c$, $\mu^* = 1$ becomes unstable and the solution bifurcates at $T = T_c$.

For the spin-$\frac{1}{2}$ ANNNI model, the inclusion of the axial second-nearest-neighbour coupling groups the spins into pairs and forces us to consider the problem as a four-state model. A pair of spins $(\alpha_{s,i}, \sigma_{s+1,i})$ can be in one of four possible states, namely $++$, $+-$, $-+$, $--$ and similarly for the adjacent pair $(\sigma_{s,i+1}, \sigma_{s+1,i+1})$. We label the four states by τ which takes values 1, 2, 3, 4, and we define

$$b_{mn} = a_{11}(\tau_i = m, \tau_{i+1} = n) \qquad m, n = 1, \ldots, 4$$

where a_{11} is the leading diagonal element of $T^{-1}(\tau_i)T(\tau_{i+1})$ where $T^{-1}AT = M$ (M is the matrix of eigenvalues).

Note that here τ_i refers to the pair of spins $(\sigma_{s+1,i}\sigma_{s,i})$ and τ_{i+1} refers to $(\sigma_{s+1,i+1}, \sigma_{s,i+1})$.

The recursion relation now involves matrices of order 4 and the recursion relation analogous to equation (9) is (Saqi and McKenzie, 1987)

$$\lambda_{s+1}A_{s+1}(\sigma_i, \sigma_j) = \begin{pmatrix} t_1\,\mathrm{e}^{3J}\lambda_1(1,1)b_{11} & t_2\,\mathrm{e}^{-J}\lambda_1(1,-1)b_{12} & t_3\,\mathrm{e}^{-J}\lambda_1(-1,1)b_{13} & t_4\,\mathrm{e}^{-J}\lambda_1(-1,-1)b_{14} \\ t_1\,\mathrm{e}^{J}\lambda_1(1,1)b_{21} & t_2\,\mathrm{e}^{J}\lambda_1(1,-1)b_{22} & t_3\,\mathrm{e}^{-3J}\lambda_1(-1,1)b_{23} & t_4\,\mathrm{e}^{J}\lambda_1(-1,-1)b_{24} \\ t_1\,\mathrm{e}^{J}\lambda_1(1,1)b_{31} & t_2\,\mathrm{e}^{-3J}\lambda_1(1,-1)b_{32} & t_3\,\mathrm{e}^{J}\lambda_1(-1,1)b_{33} & t_4\,\mathrm{e}^{J}\lambda_1(-1,-1)b_{34} \\ t_1\,\mathrm{e}^{J}\lambda_1(1,1)b_{41} & t_2\,\mathrm{e}^{-J}\lambda_1(1,-1)b_{42} & t_3\,\mathrm{e}^{-J}\lambda_1(-1,1)b_{43} & t_4\,\mathrm{e}^{3J}\lambda_1(-1,-1)b_{44} \end{pmatrix}.$$

where $\sigma_i \in \Omega_s$, $\sigma_j \in \Omega_{s+1}$ and

$$t_1(\sigma_i, \sigma_j) = \exp[2H + \sigma_i(J_2 + J) + \sigma_j J_2]$$

$$t_2(\sigma_i, \sigma_j) = \exp[\sigma_i(J_2 - J) - \sigma_j J_2]$$

$$t_3(\sigma_i, \sigma_j) = \exp[\sigma_i(J - J_2) + \sigma_j J_2]$$

$$t_4(\sigma_i, \sigma_j) = \exp[-2H - \sigma_i(J_2 + J) - \sigma_j J_2].$$

We now outline the extension to the spin-1 case. The procedure follows exactly that for the spin-$\frac{1}{2}$ case (Saqi and McKenzie 1987) except that here we have a three-state model.

As in the spin-$\frac{1}{2}$ case, we have ferromagnetic nearest-neighbour couplings and antiferromagnetic second-nearest-neighbour coupling which acts only along one axis. We take the nearest-neighbour interactions along the x and z axes to be the same.

The Hamiltonian for the Model is

$$U = \beta H \sum_{x \in V(G)} \sigma_x + \beta J \sum_{[x,y] \in E(G)} \sigma_x \sigma_y + \beta J_2 \sum_{A \subset G} \sigma_x \sigma_y$$

where $V(G)$ is the vertex set, $E(G)$ the edge set and $A = \{x, y: x, y \in V(G), d_z(x, y) = 2\}$ where d_z is the metric in the z direction. The states σ_i take values -1, 0, $+1$.

The inclusion of the axial second-nearest-neighbour coupling groups the spins into pairs and turns the problem into a nine-state model. There are nine possible configurations for a given pair of spins (σ_j, σ_i) which we denote by

$$\begin{bmatrix} + & + & + & 0 & 0 & 0 & - & - & - \\ + & 0 & - & + & 0 & - & + & 0 & - \end{bmatrix}$$

and which we label by $\tau = 1, 2, \ldots, 9$.

The method of ring recurrence allows the critical properties of a system with a classical Hamiltonian to be studied in terms of effective fields or partial partition functions, which are defined recursively. As stated earlier, in two dimensions, the effective fields are expressed as a product of matrices $A(\sigma_i, \sigma_j)$, or $A(\tau)$ and the method yields a matrix recursion relation. The matrix recursion is then reduced to a recursion between scalars; the matrices $A(\sigma_i, \sigma_j)$ are diagonalised and contributions to the product involving only the largest eigenvalues $\lambda_1(\sigma_i, \sigma_j)$ are retained. The matrices are now of the order of 9.

Following the iterative scheme described above, we define

$$b_{mn} = a_{11}(\tau_i = m, \tau_i + 1 = n) \qquad m, n = 1, 2, \ldots, 9$$

where a_{11} is the leading diagonal element of $T^{-1}AT = M$, the matrix of eigenvalues, and τ_i, $\tau_i + 1$ represent the states of two adjacent pairs of spins. The terms b_{mn} represent the weight attached to transforming the configuration of a given spin pair n into the configuration m of the adjacent spin pair under the operation of the matrix A. We denote the matrix of terms b_{mn} by $\boldsymbol{B}$.

The recursion relations are studied numerically by computing the matrices $A(\tau)$ and their eigenvalues and eigenvectors, for arbitrary initial values of $\lambda_1(\sigma_i, \sigma_j)$ and b_{mn}. The critical point is obtained from the behaviour of the fixed point of the eigenvalues $\lambda_1^*(\sigma_i, \sigma_j)$.

3. Results

Our phase diagram is shown in figure 3. We have characterised the phases by the behaviour of the normalised eigenvalues $\lambda^*(\tau)$, on iteration, where $\lambda^*(\tau) = \lambda_1(\tau)/\lambda_1(1)$, and $\lambda_1(\tau)$ is the largest eigenvalue of the matrix $A(\tau)$, and we have chosen as a norm $\lambda_1(1)$.

Upon the iteration we find for $J_2 = 0$, i.e. is with no axial second-neighbour coupling, the scheme reduces to the ordinary spin-1 Ising model as one expects. Clearly in the

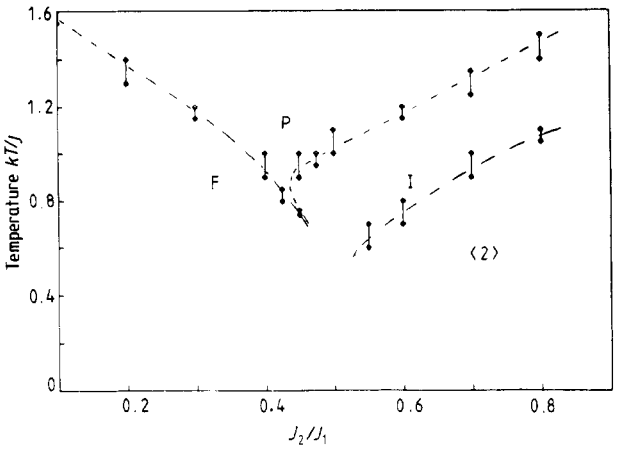

Figure 3. The phase diagram for the 2D spin-1 ANNNI model.

absence of an axial second-neighbour coupling, the states $\tau = 1, 2, 3$, are equivalent, as are states $\tau = 4, 5, 6$, and $\tau = 7, 8, 9$.

We find

$$\lambda^*(7) = \lambda^*(4) = 1 \qquad T > T_c$$

$$\lambda^*(7) \neq \lambda^*(4) \neq 1 \qquad T < T_c$$

which define T_c.

As expected, the (9×9) matrix of terms b_{mn}, denoted by $\boldsymbol{B}$, divides into blocks of size (3×3) with all the b_{mn} in a block taking the same value. The blocks along the leading diagonal have all $b_{mn} = 1$. For $T < T_c$, however, the off-diagonal blocks do not go to zero in contrast to what we would expect by analogy with the spin-$\frac{1}{2}$ Ising model.

For $J_2 \neq 0$ we find four phases.

(i) *The paramagnetic phase.* Here we find points such that the eigenvalue associated with a given state τ is equal to that associated with the complementary state τ', which is obtained by interchanging + and − spins

$$\lambda^*(\tau) = \lambda^*(\tau').$$

Thus for example $\lambda^*(3) = \lambda^*(7)$ where $\tau = 3$ is the state $\binom{+}{-}$ and $\tau = 7$ is state $\binom{-}{+}$.

The b_{mn} are such that

$$b_{mn} = b_{m'n'}$$

where m', n' are complementary states to m, n. This means, for example, $b_{27} = b_{83}$, remembering that $b_{mn} = a_{11}(m, n)$.

(ii) *The ferromagnetic phase.* Here we find

$$\lambda^*(\tau) \neq \lambda^*(\tau')$$

and in general all the eigenvalues converge to different fixed points. We find also

$$b_{mn} \neq b_{m'n'}.$$

(iii) *The '++−−' phase.* The eigenvalues $\lambda^*(\tau)$ iterate to a 2-cycle. However, as with the spin-$\frac{1}{2}$ ANNNI model (Saqi and McKenzie 1987), each step in our iterative scheme takes into account two rows of the square lattice, and so the 2-cycle corresponds

to a $++--$ phase. In this phase those b_{mn} associated with a configuration that has an up $(+)$ spin adjacent to a down $(-)$ spin along the same row, are zero. thus for example b_{16} (corresponding to $^{+0}_{+-}$) and b_{18} (corresponding to $^{+-}_{+0}$) are both zero. This suggests that this phase is in fact a $++--$ phase with two rows of predominantly 'up' spins followed by two rows of mainly 'down' spins, but with the possibility of 0-spin states occurring within a given row. Since the only interaction along a row (along the x axis in figure 1) is the ferromagnetic nearest-neighbour interaction, it would be energetically unfavourable for spins to align with a $+$ spin adjacent to a $-$ spin along a given row.

(iv) *The incommensurate phase.* Here, the eigenvalues do not converge to a fixed point but describe an oscillatory chaotic-like behaviour. No regular behaviour has been found for the b_{mn}, although the possibility of some long-period cyclic behaviour exists.

The phase idagram in figure 3 was obtained by increasing the temperature for fixed values of $-J_2/J$ and observing the behaviour of the eigenvalues on iteration.

The phase diagram is generally similar to that of the spin-$\frac{1}{2}$ ANNNI model (Saqi and McKenzie 1987). The critical temperatures for a given competing strength $-J_2/J$ are lower than for the corresponding spin-$\frac{1}{2}$ case. We observe that the effect found in our study of the spin-$\frac{1}{2}$ ANNNI model, whereby the phase boundary between the incommensurate and paramagnetic phases moves slightly to the left of the line $-J_2/J = 0.5$ before returning to $J_2/J = 0.5$ as T decreases, is now more apparent. The error bars in figure 3 indicate the uncertainty in pinning down the phase boundaries. The lower points on the error bars indicate definite evidence for one phase and the upper points indicate the presence of the other phase. We find that, for values of $-J_2/J_1 < 0.5$, as the temperature is increased the phases change from ferromagnetic to paramagnetic, then to incommensurate and then to paramagnetic, and there are clear regions of incommensurate behaviour. We believe this to be a real effect and not an artefact of the method of ring recurrence. Incommensurate states are found to exist for $-J_2/J$ as low as 0.45. Numerical evidence suggests that there is no multicritical point and that the paramagnetic phase extends down to $T = 0$, as was found with our study of the spin-$\frac{1}{2}$ ANNNI model.

The phase boundaries are obtained by increasing the temperature for fixed values of $-J_2/J_1$, and observing the behaviour of the eigenvalues on iteration. Very near the phase boundary a longer time is required for convergence. The CPU time depends on how precisely the phase boundaries are located. The implementation of the method of ring recurrence to obtain the phase diagram in figure 3 took only a few hours on a VAX 11/750 computer. We finally observe that it would be straightforward to calculate the behaviour of the wavevector q (Vannimenus 1981) in the incommensurate phase using our iterative scheme. An accurate calculation of q would require large numbers of iterations and, due to the size of the matrices $A(\tau)$, would take considerably more computing than was needed for the spin-$\frac{1}{2}$ ANNNI model.

We observe also that the method can be extended to the biaxial case, for which a real space renormalisation group study has recently been reported. (Aydın and Yalabık 1989). Here we would group the spin in clusters of four and each state τ would represent $(\sigma_{s,i}, \sigma_{s+1,i}, \sigma_{s,i+1}, \sigma_{s+1,i+1})$. Hence the matrices $A(\tau)$ would be of order 16. We expect interesting properties of the phase diagram to be revealed by such a study. The method of ring recurrence provides a useful way of investigating the phase diagram of fairly complex models and can be implemented without requiring excessive computer resources.

Appendix. Elements of the matrix $A(\sigma_k, \sigma_l)$ for the spin-1 ANNNI model

We list below the elements of the matrix $A(\sigma_k, \sigma_l)$. The system is described by a set of nine matrices, each of size (9*9) corresponding to the possible configurations. Let the elements of $A(\sigma_k, \sigma_l)$ be a_{ij} (σ_k, σ_l) and let $a_{ij} = z_j(\sigma_k, \sigma_l)a'_{ij}$ where

$$z_1 = \exp(H + \sigma_k(J + J_2) + \sigma_l J_2) \exp(J)$$

$$z_2 = \exp(H + \sigma_k J_2)$$

$$z_3 = \exp(\sigma_k(J_2 - J) - \sigma_l J_2) \exp(-J)$$

$$z_4 = \exp(H + \sigma_k J + \sigma_l J_2)$$

$$z_5 = 1$$

$$z_6 = \exp(-H\sigma_k J - \sigma_l J_2)$$

$$z_7 = \exp(-\sigma_k(J - J_2) \exp(-J)$$

$$z_8 = \exp(-H - \sigma_k J_2)$$

$$z_9 = \exp(-2H - \sigma_k(J + J_2) - \sigma_l J_2)$$

and σ_k, σ_l can take values -1, 0, $+1$.

The elements a'_{ij} are given by the following matrix below:

$$\begin{bmatrix}
e^{2J} & e^{J} & 1 & e^{J} & 1 & e^{-J} & 1 & e^{-J} & e^{-2J} \\
e^{J} & e^{J} & e^{J} & 1 & 1 & 1 & e^{-J} & e^{-J} & e^{-J} \\
1 & e^{J} & e^{2J} & e^{-J} & 1 & e^{J} & e^{-2J} & e^{-J} & 1 \\
e^{J} & 1 & e^{-J} & e^{J} & 1 & e^{-J} & e^{J} & 1 & e^{-J} \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
e^{-J} & 1 & e^{J} & e^{-J} & 1 & e^{J} & e^{-J} & 1 & e^{J} \\
1 & e^{-J} & e^{-2J} & e^{J} & 1 & e^{-J} & e^{2J} & e^{J} & 1 \\
e^{-J} & e^{-J} & e^{-J} & 1 & 1 & 1 & e^{J} & e^{J} & e^{J} \\
e^{-2J} & e^{-J} & 1 & e^{-J} & 1 & e^{J} & 1 & e^{J} & e^{2J}
\end{bmatrix}.$$

This defines the matrices $A(\sigma_k, \sigma_l)$, which we use in the iterative scheme to locate the critical points.

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