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LETTER TO THE EDITOR

Branching processes in the ANNNI model

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Abstract. The mean-field equations of the simple cubic ANNNI model are studied on finite lattices. The results are consistent with the sequence of distinct commensurate phases, $\langle 2^{k-1}3\rangle$, $k = 1,2,3,\ldots$, springing from the multiphase point, found using low-temperature series expansions. Moreover, evidence for new structure combination branching processes is presented, which generate phases of type $\langle (2^l3)^m(2^{l+1}3)^n\rangle$ or $\langle (23^l)^m(23^{l+1})^n\rangle$, where l, m and n are integers.

The axial next-nearest neighbour Ising (or ANNNI) model (Fisher and Selke 1980) is one of the simplest statistical mechanical models to exhibit complex spatially modulated phases. It is composed of spin-$\frac{1}{2}$ Ising variables, $S_i = \pm 1$, situated on a regular d-dimensional lattice formed of $(d-1)$-dimensional layers of coordination number $q_\perp$ normal to the z axis. Within the layers each spin is coupled only by nearest-neighbour ferromagnetic interactions, $J_0 > 0$. However, along the z axis, spins are coupled by competing nearest, $J_1 > 0$, and next-nearest neighbour, $J_2 = -\kappa J_1 < 0$, interactions. The parameter κ thus controls the degree of competition.

The model is known (as reviewed by Bak (1982), Fisher and Huse (1982) and Selke (1983)) to form a low-temperature ferromagnetic phase for $\kappa < \frac{1}{2}$, and a $\langle 2\rangle$ phase for $\kappa > \frac{1}{2}$. At low temperatures, for $d > 2$ and $4J_0 > J_1$, the wedge in the (κ, T) phase diagram between these two phases is filled by a countably infinite sequence of discrete commensurate phases, $\langle 2^{k-1}3\rangle$, $k = 1,2,3,\ldots$, springing from the multiphase point ($\kappa = \frac{1}{2}$, $T = 0$) (Fisher and Selke 1980, 1981). (For applications of the techniques to ANNNI models in a field, see Pokrovskii and Uimin (1982 a, b), Smith and Yeomans (1982) and Uimin (1982, 1983).) $\langle 2^{k-1}3\rangle$ denotes a periodic structure, where $(k-1)$ pairs of lattice layers pointing (predominantly) two 'up' ($S_i = +1$) and two 'down' ($S_i = -1$) are followed by three layers all pointing (predominantly) in the same direction. Accordingly, the wavevector, q, varies at fixed temperature, with κ in *discrete* steps, $q_k = \pi k/(2k+1)a$; a is the lattice constant.

On the other hand, close to the boundary of the modulated phase to the paramagnetic phase the wavevector is believed to change *continuously* with κ, as has been shown using linearised mean-field theory (Elliott 1961), high-temperature series expansion (Redner and Stanley 1977, Oitmaa 1983), and in agreement with Monte Carlo results (Selke and Fisher 1979, 1980).

To explore the region in between the discrete low-temperature phases of type $\langle 2^{k-1}3\rangle$ and the structures with continuously changing wavevector close to T_c, one apparently has to rely upon approximate methods, in particular mean-field theories.

The results of previous such calculations can be summarised as follows. (a) Iterated mapping techniques (Jensen and Bak 1983) have suggested the existence of a definite, κ-dependent, temperature below which incommensurate structures are of measure zero—in analogy with the breaking of analyticity investigated by Aubry (1981, 1983). (b) Finite lattice mean-field calculations (Bak and von Boehm 1980) found in addition to phases of the form $\langle 2^{k-1}3\rangle$ some different commensurate structures.

However, these results, albeit very interesting, do not give a coherent description of that intermediate region. The purpose of this letter is to present results of a *systematic* finite lattice mean-field calculation. As a result, strong evidence is given for non-zero temperature branching processes which generate phases of the form $\langle (23^l)^m(23^{l+1})^n\rangle$ and $\langle (2^l3)^m(2^{l+1}3)^n\rangle$, l, m, n, integers, and which proceed via a simple structure combination process.

We consider the mean-field equations (Bak and von Boehm 1980) of the simple cubic or tetragonal ANNNI model

$$M_i = \tanh(\beta(4J_0M_i + J_1(M_{i+1}+M_{i-1}) - \kappa J_1(M_{i+2}+M_{i-2})) \qquad (1)$$

where $\beta = 1/k_BT$; M_i is the magnetisation of the ith layer along the z direction. We take $J_0 = J_1$. To determine the stable magnetisation pattern at a given set of values κ and k_BT/J_0 one compares the free energies of solutions to equations (1) with periodic boundary conditions for various lattice sizes, i.e. number of layers, N. The solutions were obtained iteratively. In principle, one should consider all integers, N, using numerical routines with arbitrarily high precision. Obviously this is not feasible, and one has to restrict the analysis to a reasonably chosen variety of lattice sizes. Previous studies (von Boehm and Bak 1979, Yokoi *et al* 1981, Rasmussen and Knak Jensen 1981, Öttinger 1983) considered all lattice sizes up to a certain maximal value, usually of the order of 20. Thereby one easily loses the long wavelength structures. Here, we suggest and carry out the following, different, self-consistent approach. We guess that at low temperatures new phases are generated by a 'structure combination branching process', i.e. that two adjacent phases, $\langle A\rangle$ and $\langle B\rangle$, produce the new phase $\langle AB\rangle$ at a definite branching point. This process may be repeated, as one increases the temperature, to form more and more complicated commensurate phases ($\langle AAB\rangle$, $\langle ABB\rangle$, $\langle A^3B\rangle, \ldots$). (If such a process continued indefinitely, one would obtain a complete devil's staircase in Aubry's (1981) terminology.) Accordingly, we compared structures of the type $\langle A^nB^m\rangle$, n, m integers, where A and B are low-temperature phases known from the low-temperature series expansion. The actual structures that we always compared are $\langle 2^{k-1}3\rangle$, $k \leqslant 5$, and the ones listed in table 1, consistent with assumed monotonicity in q with κ at fixed T. It would be, of course, desirable to include combinations of even higher order and larger values of k. However, the corresponding analysis close to the multiphase point is beyond the numerical precision available to us (128 bits).

The results confirm the hypothesis of a structure combination branching process, see figure 1. The branching points of the combinations of lower order occur at lower temperatures than the ones of higher order. In table 1, we list all the branching points that we have found. The corresponding phase diagram is depicted in figure 1. Note that the κ scale is schematic. We observed up to three consecutive structure combinations, e.g. $\langle (23^2)(23)^2\rangle$. It remains an open question whether this structure combination process (which might also be considered as a bifurcation) continues to indefinitely high order, before the truly incommensurate structures may set in. It should be mentioned

Table 1. Branching temperatures for structure combination phases in the ANNNI model.

Branching structure	Branching temperature
$\langle 23^4 \rangle$	1.985 ± 0.005
$\langle 23^3 \rangle$	1.537 ± 0.005
$\langle 23^2(23^3) \rangle$	1.635 ± 0.005
$\langle 23^2 \rangle$	$0.851\,925 \pm 0.000\,005$
$\langle 23(23^2)^2 \rangle$	1.0 ± 0.1
$\langle 23(23^2) \rangle$	0.882 ± 0.005
$\langle (23)^2 23^2 \rangle$	1.075 ± 0.005
$\langle (23)^2 2^2 3 \rangle$	0.95 ± 0.05
$\langle 23(2^2 3) \rangle$	0.66 ± 0.02

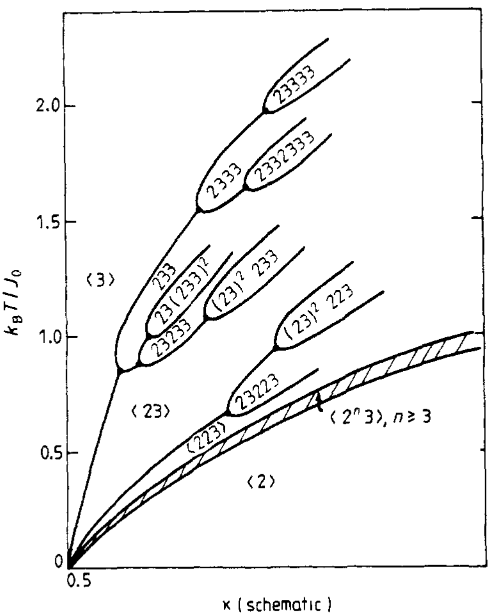

Figure 1. The low-temperature phase diagram of the ANNNI model. The temperature axis is to scale, the κ axis is schematic.

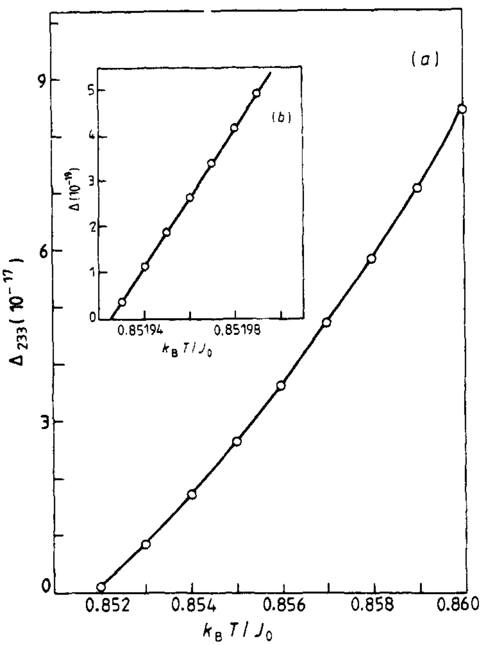

Figure 2. The widths of the $\langle 233 \rangle$ phase against temperature. (*b*) gives an enlarged view near the branching temperature.

that our data on the $\langle 2^{k-1}3 \rangle$ boundaries confirmed quantitatively the low-temperature series results (Fisher and Selke 1981).

We also addressed the question whether there is a characteristic asymptotic behaviour near the branching points. An example is shown in figure 2. One finds that the width, Δ, of the $\langle 233 \rangle$ phase (see figure 1) vanishes asymptotically in a linear fashion, as one approaches the branching temperature, T_B. Over a wide range of temperatures one obtains $\Delta \sim A(T - T_B)\exp(-a/k_B T)$. Results of systematic studies on this asymptotic behaviour as well as finite lattice calculations on the ferromagnetic side, $\kappa < \frac{1}{2}$, of the model, consistent with an apparently continuously changing wave-vector, will be published elsewhere (Duxbury and Selke 1983).

Summarising, we conclude that we have found evidence for a new *structure combination* branching process at low temperatures (where mean-field theory is expected to be correct) in the ANNNI model.

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