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Critical behaviour of the two-dimensional biaxial next-nearest-neighbour Ising model. A Monte Carlo study

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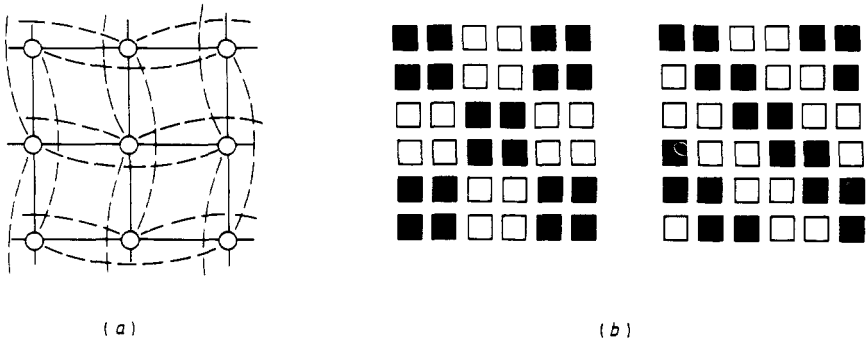
Abstract. The critical behaviour of an Ising model with competing interactions along both axes of a square lattice (the BNNNI model) is investigated by Monte Carlo methods. Convincing evidence for the existence of modulated structures near the transition(s) is obtained but the form of the phase diagram remains unclear.

1. Introduction

In two recent papers (Oitmaa and Velgakis 1987, Oitmaa *et al* 1987) we investigated the nature of the phase transitions and phase diagram of a particular type of two-dimensional Ising model. This model, which we termed the biaxial next-nearest-neighbour Ising model or BNNNI model, has competing nearest- and next-nearest-neighbour interactions along both axes of a square lattice, as shown in figure 1(*a*).

Ising models with competing interactions have been found to exhibit rich and complex phase diagrams, with a variety of ordered phases at low temperatures, including spatially modulated phases (Selke 1984). The nature of the phase transition can also vary quite dramatically, with the occurrence, in particular cases, of non-universal behaviour, first-order transitions and multicritical points. A model which has been much studied in this context is the ANNNI model. The model studied in this paper can be thought of as an isotopic version of the ANNNI model.



(*a*) (*b*)

Figure 1. (*a*) The interactions of the two-dimensional BNNNI model. (*b*) The two types of ground state for $J' < -\frac{1}{2}|J|$.

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The Hamiltonian of the model is

$$H = -J\sum_{\langle ij\rangle} s_i s_j - J'\sum_{[ij]} s_i s_l \qquad s_i = \pm 1 \tag{1}$$

where the summations are over nearest- and next-nearest-neighbour pairs along both lattice directions. Because the free energy in zero field is an even function of J, we choose this interaction to be ferromagnetic ($J>0$). The other interaction can have either sign. Of greatest interest is the region $J' < -\frac{1}{2}|J|$, where the ground state is either of the 'chessboard' or 'staircase' type, as shown in figure 1(b). The nature of the transition, or transitions, from this ordered phase to the high-temperature disordered phase remains uncertain. Early Monte Carlo work (Hornreich *et al* 1979, Selke and Fisher 1980) suggested a sequence of two transitions: a transition from the commensurately modulated chessboard phase to an intermediate incommensurate phase, followed by a Kosterlitz–Thouless transition to the disordered phase. However, the more recent Monte Carlo study of Landau and Binder (1985) suggests that there is no intermediate phase; rather, the commensurate and disordered phases are separated by a single first-order transition.

Our previous work on this model using series methods (Oitmaa and Velgakis 1987) and transfer matrix calculations (Oitmaa *et al* 1987) was unable to resolve this discrepancy. Both approaches did give some indication that the two-transition picture was perhaps the correct one, but the results could not be interpreted unambiguously. We were thus led to continue our studies of this, at first glance simple but apparently quite subtle, model, this time using Monte Carlo methods.

The arrangement of the paper is as follows. In § 2 we briefly discuss our methods, and present results for the internal energy as a function of temperature. These results, for relatively large lattices, do not support the picture of a single first-order transition. We find evidence for the existence of a sequence of intermediate states, and in § 3 we attempt to characterise the nature of these. Finally, in § 4 we summarise our results and present our conclusions.

2. The internal energy

The general ideas and the technical details of Monte Carlo simulations are well known and documented, so we will not repeat these at length. We have found the article by Binder and Stauffer (1984) particularly helpful, and recommend it to others embarking on Monte Carlo calculations for the first time.

We have considered $N \times N$ Ising systems, described by the Hamiltonian (1), on a square lattice with periodic boundary conditions. Our computer program allows us to choose a starting configuration which is disordered ('hot' start) or ordered ('cold' start). A sequence of configurations is then generated via the standard Metropolis importance-sampling algorithm. Spins are chosen randomly for flipping, and a 'sweep' (more usually called a MCS/spin) corresponds to a sequence of N^2 tests, i.e. on average each spin is chosen once per sweep. This defines a 'timescale' for the simulation. The configurational properties of the system are then 'measured' (i.e. computed) for a sequence of time steps and thermodynamic quantities obtained as sample averages of the resulting time series $\{X_i\}$

$$\langle X\rangle = \frac{1}{n}\sum_{i=1}^{n} X_i.$$

In order to reduce correlations between successive measurements we have chosen to make a measurement after every NBLOCK sweeps, where typically NBLOCK = 25.

In all of the work reported here we have chosen the ratio of parameters $J'/J = -1$, a point which lies well within the 'modulated' region of the phase diagram. For this particular value Landau and Binder (1985) give a temperature of $k_B T/J \simeq 1.4$ for the first-order transition, obtained for a 48×48 lattice.

Our first runs were carried out on a 40×40 lattice, to try to reproduce the Landau-Binder results. In figure 2 we show results of two runs, in the form of energy time series, for $K = J/k_B T = 0.675$. The upper graph, corresponding to an initial disordered configuration, settles down quickly to a mean energy of approximately -1.72 whereas the lower graph, corresponding to an initial ordered state, settles down to a mean energy of approximately -1.95. Clearly at this temperature there are two quasi-equilibrium states, a situation characteristic of a system which undergoes a first-order transition. By carefully heating or cooling the system it is possible to follow either of these states into a temperature regime where they are clearly not the absolute equilibrium state, but merely metastable. Based on a large number of runs of this type, we obtain the variation of internal energy with temperature shown in figure 3(*a*), which supports the picture of a first-order transition in the region $K \simeq 0.7$. To verify this, and to locate the transition temperature more accurately, we have integrated the internal energy to obtain the free energies for the high- and low-temperature branches as discussed by Binder and Stauffer (1984). The two free-energy branches, shown in figure 3(*b*), clearly intersect with different slopes at $K \simeq 0.65$. This apparently confirms the Landau-Binder conclusion, namely a first-order transition, albeit at a slightly higher temperature, $k_B T/J \simeq 1.54$.

In order to confirm these conclusions, and to see if the transition temperature showed any significant size dependence, we decided to carry out further runs on larger lattices, first 80×80 and subsequently 120×120. The strategy adopted was the same

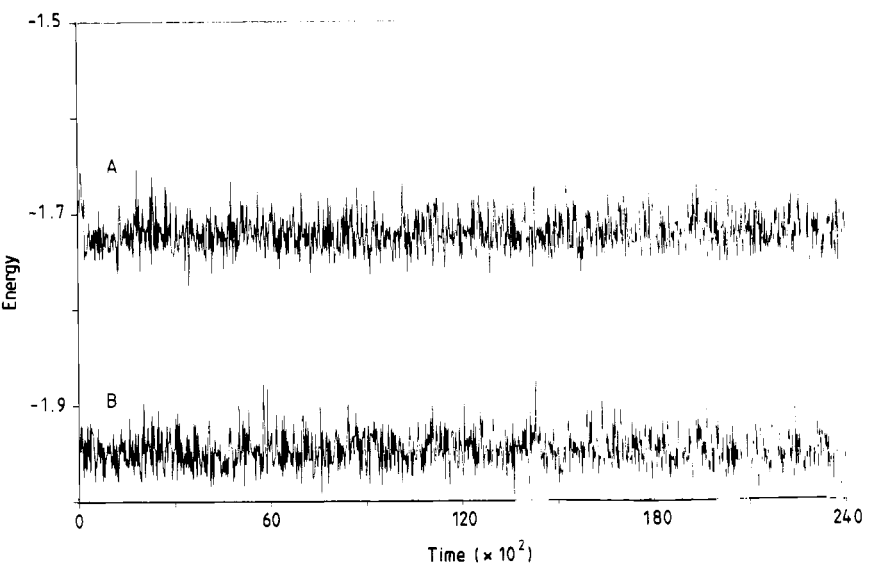

Figure 2. Energy time series for the 40×40 lattice for temperature $K = 0.675$. The two graphs correspond to (A) hot and (B) cold starts and illustrate the two stable or quasi-stable states at this temperature.

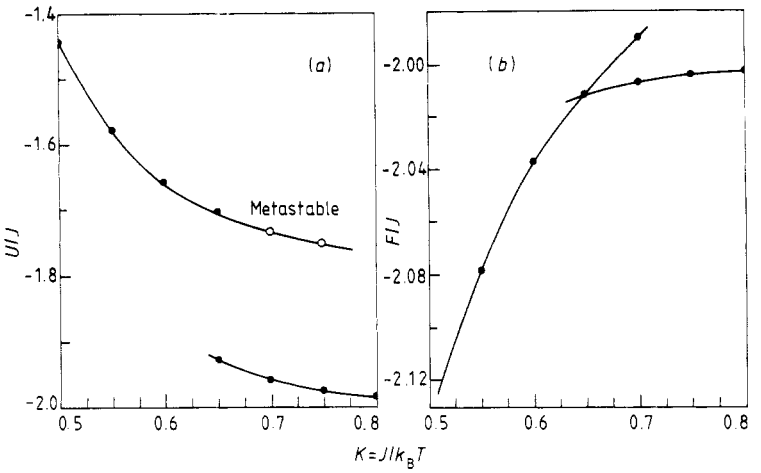

Figure 3. (*a*) Internal energy against temperature for the 40×40 lattice, showing two distinct energy branches. (*b*) The free energies of the two branches, intersecting with different slopes at $K \simeq 0.65$.

as before, namely to look very closely at the time series for the energy and to identify equilibrium or quasi-equilibrium states. In all cases we have used rather long runs of up to 30 000 sweeps. Our results suggest that the true picture is more complex than that described above. In particular, for the 80×80 lattice we have obtained strong evidence for the existence of an intermediate state, which we believe to be thermodynamically stable over a certain temperature range. In figure 4 we show the time series for the energy, for two runs, both corresponding to $K = 0.650$. The upper trace is for a system, initially in a disordered state, which has been allowed to cool slowly,

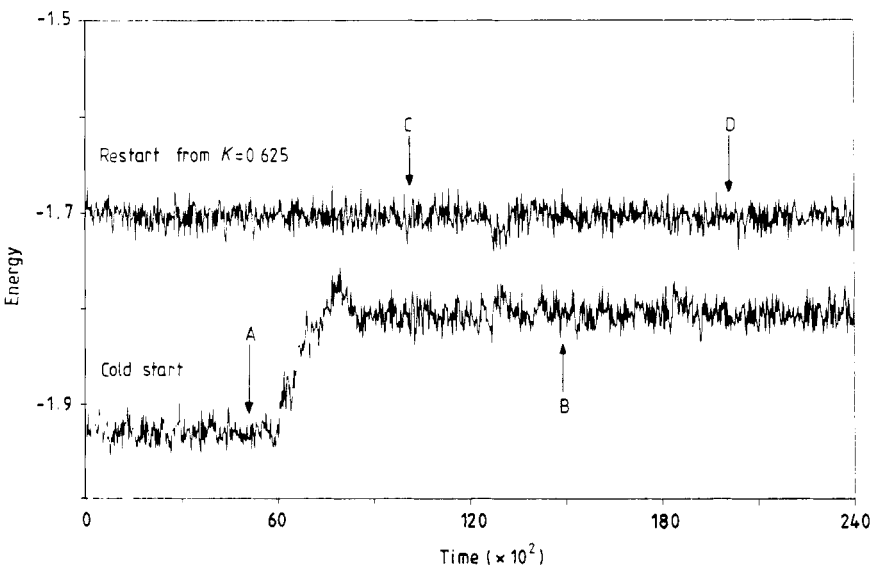

Figure 4. Energy time series for the 80×80 lattice for temperature $K = 0.650$. The upper trace corresponds to point P in figure 5, the lower trace to point R, relaxing to point Q.

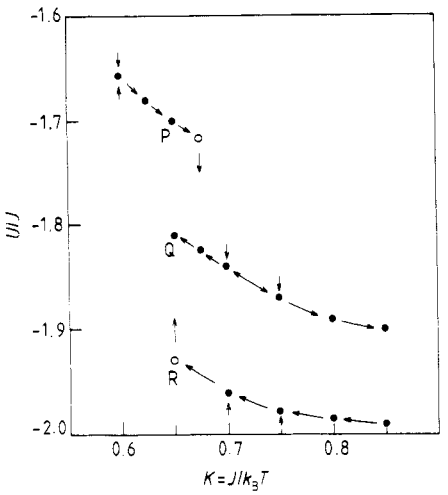

Figure 5. Internal energy against temperature for the 80×80 lattice, showing three distinct energy branches. The points P, Q, R refer to the text and to figure 4. The arrows indicate the manner in which a particular state was reached, i.e. from a hot start, cold start or restart from a previous point. The open circles denote unstable points.

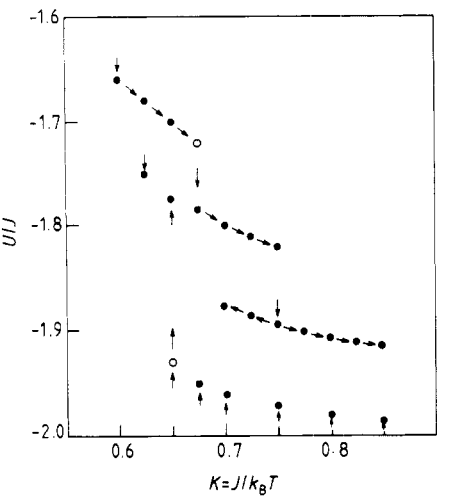

Figure 6. Internal energy against temperature for the 120×120 lattice, showing four energy branches. The open circles denote unstable points.

through a sequence of intermediate temperatures. This corresponds to point P in figure 5. We believe that this state is metastable, since a hot start at this temperature takes the system to the intermediate state (point Q in figure 5). The lower trace shows the system, started in an ordered configuration, initially reaching a quasi-equilibrium state with energy -1.93 (point R in figure 5), but then spontaneously relaxing to a higher energy state (point Q in figure 5) which appears to be the stable state at this temperature. Figure 5 shows the plot of internal energy against temperature for the 80×80 lattice, with three distinct energy branches. Similar runs for a 120×120 lattice show four distinct energy branches, as shown in figure 6. In this case there appear to be two intermediate states, each of which appears to be stable over a finite temperature range.

While these results clearly indicate that the behaviour of the model is rather unusual, the intepration is not entirely clear. In the following section we attempt to identify the nature of the intermediate phase(s).

3. The nature of the phases

Our Monte Carlo runs for the 80×80 lattice, reported in the previous section, indicate the possible presence of a stable intermediate state. In order to try to understand the nature of this state, if it exists, we have followed two approaches.

The first is to look carefully at the spin configurations themselves to try to discern an apparent pattern. Figure 7 shows four such configurations, corresponding to the points A, B, C and D in the time series (figure 4). The first configuration, corresponding to the lowest energy branch, is clearly a chessboard phase with a small number of isolated defects. The second configuration, corresponding to the intermediate branch,

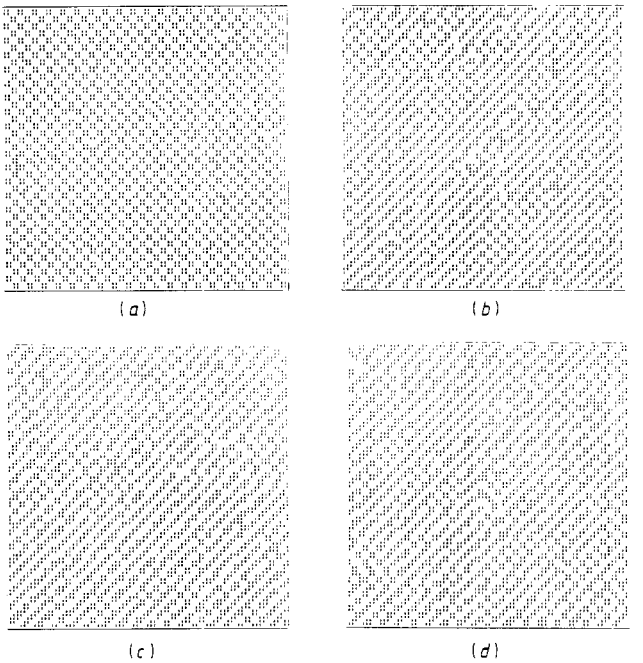

Figure 7. Spin configurations for the 80×80 lattice. (a), (b), (c), (d) correspond to the points A, B, C, D in the energy time series of figure 4.

consists of regions of chessboard-like order indispersed with regions of staircase-like order. In addition there are many 'three-spin' groups, consisting of three adjacent spins all up or all down. These appear to be the main mechanism which is breaking up the ordered phases. A similar process has been observed in the two-dimensional ANNNI model (Selke 1981), although the present case is more complicated since the three-spin groups occur along both lattice directions. The last two configurations both correspond to the highest energy branch. The number of three-spin groups is significantly larger and other types of composite defect structures appear. There is, however, qualitative similarity between these configurations and the intermediate-state configuration.

A tentative explanation of what is happening can be given in terms of these three-spin groups. The fully ordered chessboard and staircase structures have a wavevector $q=2\pi(\frac{1}{4},\frac{1}{4})$ in the diagonal direction. To disturb the structure only locally, it is necessary to create three-spin groups in multiples of four along each row or column of the lattice. For the 80×80 lattice the intermediate state appears to be a staircase plus four three-spin groups and the higher state a staircase plus eight three-spin groups. These changes in configuration give rise to jumps in the energy and in the wavevector. The change in wavevector, in either direction, is $\Delta q=2\pi m/4N$ where m is the number of three-spin groups.

This picture is confirmed by looking at the Fourier coefficients of the magnetisation for diagonal rows. We follow the method used by Selke and Fisher (1979) for the ANNNI model. The magnetisation per diagonal row can be written as

$$M(z)=\sum_{k=1}^{N}\left[a_k\cos\left(\frac{2\pi kz}{N}\right)+b_k\sin\left(\frac{2\pi kz}{N}\right)\right] \tag{2}$$

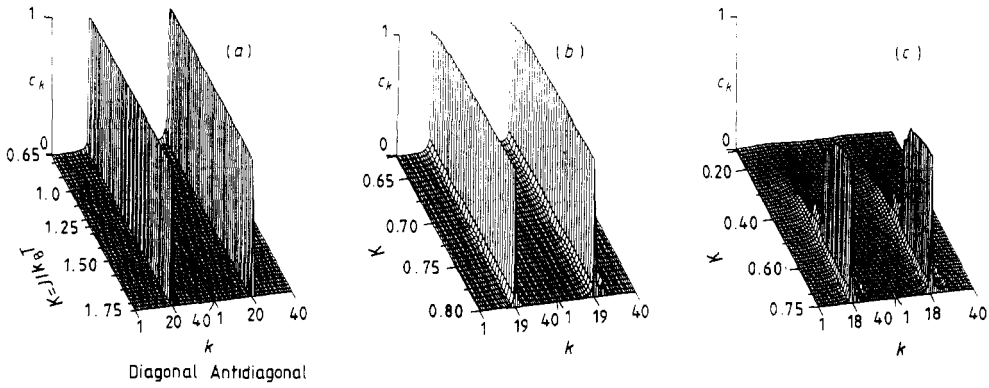

Figure 8. Fourier coefficients of the diagonal magnetisation against temperature and wavenumber for the three energy branches of the 80×80 lattice (a), lowest branch; (b), middle branch; (c), upper branch.

where $z = 1, 2, \ldots, N$ is a discrete index labelling the diagonal rows. For each of the three energy branches of the 80×80 lattice, shown in figure 5, we have computed the quantities $c_k = (a_k^2 + b_k^2)^{1/2}$ as a function of k. These are plotted in figure 8(a), (b) and (c) for both sets of diagonals. Figure 8(a), corresponding to the lowest state, shows c_k sharply peaked at $k = 20$, i.e. $q = 2\pi/4$. This is the wavenumber which describes the chessboard or staircase ground states, and hence this energy branch corresponds to the ordered phase of the system. Figure 8(b), corresponding to the middle state, shows c_k peaked at $k = 19$. This corresponds to a wavenumber $q = 38\pi/80$, i.e. a change in wavenumber of $2\pi/80$, in agreement with the picture of four three-spin groups discussed above. Figure 8(c), which corresponds to the upper branch, shows no peak in c_k at high temperatures, and the development of a peak at $k = 18$ as the temperature is lowered. This signifies the development of an ordered state with $q = 36\pi/80$, i.e. $\Delta q = 4\pi/80$, in agreement with the picture of eight three-spin groups.

Although we have not calculated the Fourier coefficients of the magnetisation for the 120×120 lattice, we surmise that the four energy branches we have observed correspond respectively to 0, 4, 8, 12 groups of three-spins.

4. Conclusions

By means of careful Monte Carlo studies on rather large lattices we have studied the nature of the phase diagram of the biaxial next-nearest-neighbour Ising model, or BNNNI model, for the ratio of interactions $J'/J = -1$. This corresponds to the region in which the ground state of the system is a modulated structure with wavevector $q = 2\pi(\frac{1}{4}, \frac{1}{4})$, the 'chessboard' or 'staircase' configurations.

Recently, Landau and Binder, also using Monte Carlo techniques, concluded that the model has a single first-order transition between the ordered and disordered phases. Our results suggest that the true picture is more complicated. For 80×80 and 120×120 lattices we find evidence for a sequence of modulated structures, associated with discrete jumps in the wavevector. These discrete jumps in the wavevector also correspond to discrete jumps in the internal energy, which at first sight might be interpreted

as a sequence of first-order transitions. However, as the lattice size increases these jumps become smaller, and in the thermodynamic limit the internal energy may well be a continuous function of temperature.

Our results still do not unambiguously determine the behaviour of this model, as they are consistent with a number of possible scenarios, for example

(i) a single continuous transition;

(ii) two transitions separated by an intermediate floating phase; or

(iii) a 'devil's staircase' type of structure.

We propose to continue these studies to try to distinguish between these various possibilities.

Acknowledgments

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