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Antiferromagnetic Ising model on the Penrose lattice

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Abstract. We use Monte Carlo techniques to study the antiferromagnetic Ising model on the two-dimensional Penrose lattice. Two types of interaction are included, resulting in subtle frustration effects and a rather complex phase diagram.

1. Introduction

The subject of quasi-crystals, their structure and physical properties, is an active area of current research. These systems are of considerable interest in themselves, but are also important in providing a bridge between regular periodic structures and the fully disordered or amorphous state. For the uninitiated, the book by Steinhardt and Ostlund (1989) contains most of the significant early papers on the subject as well as excellent summaries.

In this paper we address the question of magnetic-order and magnetic-phase transitions in quasi-crystals, using as a specific system the Ising model on the two-dimensional Penrose lattice. In figure 1(a) we show a portion of the Penrose lattice, which is a non-periodic tiling of the plane with two kinds of rhombus, a fat one with angles of 72° and 108° and a thin one with angles 36° and 144°. Our model then has Ising spins $\sigma = \pm 1$ at all of the vertices of the Penrose lattice.

There has been some previous related work. An important and immediate question is whether the model has a phase transition in the same universality class as for regular two-dimensional lattices. That this is indeed the case has been demonstrated for the ferromagnetic Ising model by Bhattacharjee *et al* (1987) and by Okabe and Niizeki (1988) and for the Potts model by Wilson and Vause (1988). For antiferromagnetic interactions frustration effects may occur and potentially new kinds of ordered states and transitions may exist. It is clear that if the antiferromagnetic interactions in the model occur only along the rhombus edges then this is a bipartitite structure, i.e. it

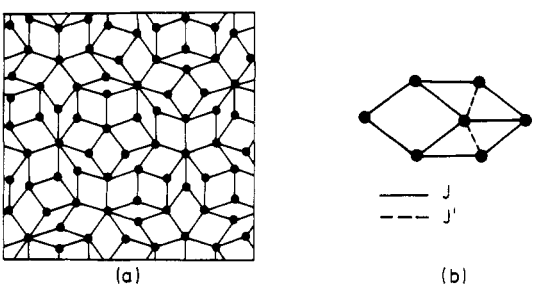

Figure 1. (a) The Penrose lattice. (b) The two interaction types J and J'.

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can be divided into two sublattices in the same way as, for example, the square lattice. It will thus support a simple antiferromagnetic ordered phase and furthermore there is a complete correspondence between the ferromagnetic and antiferromagnetic states. However, if additional interactions are permitted then this will no longer be the case.

We consider in this work a model with two kinds of interaction, both antiferromagnetic and of strengths J and J'. This is shown in figure 1(b) and corresponds to the physically reasonable assumption that significant exchange is present for the two smallest interatomic spacings in the structure. Our Hamiltonian is then

$$\mathcal{H} = J \sum_{\langle ij \rangle} \sigma_i \sigma_j + J' \sum_{[ij]} \sigma_i \sigma_j \tag{1}$$

where the first summation is over rhombus edges and the second is over the short diagonals of thin rhombi. We do not consider the case of an external magnetic field, which would certainly be of interest also.

It is easy to see that frustration effects can occur in this structure. For certain ratios of J'/J some spins can become completely free, provided the remaining lattice remains antiferromagnetic. This is shown in figure 2, and may result in an overall ground state with non-zero entropy. Furthermore it is plausible that a large number of different configurations may exist with energies equal to or nearly equal to the global minimum—a situation reminiscent of spin-glasses. Thus we might expect to find evidence for a complex phase space with many local energy minima, metastable states and long relaxation times, and perhaps the absence of a true equilibrium phase transition. Our motivation to study this problem was partly provided by such considerations.

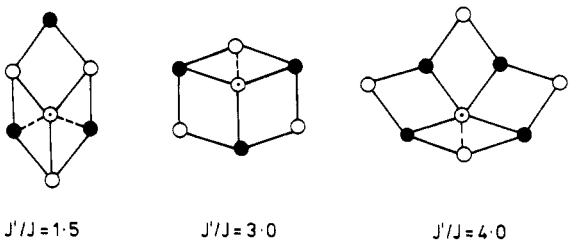

Figure 2. Local fully frustrated structures in an antiferromagnetic background. Spins are shown as ● (up) and ○ (down). In each case the central spin ⊙ is free to be either up or down with no change in energy.

Our approach to the problem is via Monte Carlo simulations, as in most of the previous work. The Monte Carlo method has the advantage that it can provide rather direct evidence for the existence of complex ordered states and for identifying true equilibrium states. It is able to handle non-periodic structures with no extra difficulty. The method is by now standard in this field but a useful source for unfamiliar readers is the book by Binder (1984). In the next section of the paper we will discuss some of the more technical aspects of our work. In section 3 we present and discuss the main results, and finally in section 4 we summarize our conclusions.

2. Technical details

The essence of the Monte Carlo method is to generate a succession of configurations of the system, in a stochastic manner but one which samples states in accordance with

the Boltzmann distribution. Our computer program allows us to choose a starting configuration which is random or ordered, or to restart from the final configuration of a previous run. Spins can be chosen either sequentially or randomly for updating, and a complete pass through the lattice, or 'sweep', defines the unit of 'time' for the simulation. The physical variables, such as energy and order parameters, are then 'measured', i.e. computed for a sequence of time steps and thermodynamic quantities are obtained as averages of the resulting time-series $\{X_i\}$

$$\langle X\rangle = \frac{1}{M}\sum_{i=1}^{M} X_i. \tag{2}$$

In order to reduce correlations between successive measurements, we have chosen to make a measurement after every ten sweeps. Individual runs are typically of length 10^5 sweeps, with the initial measurements discarded. In some cases longer runs have been made. Our Monte Carlo program automatically computes, for each run, the average energy $\langle E\rangle$, which is to be identified with the thermodynamic internal energy, the specific heat

$$C = \frac{1}{k_B T^2}(\langle E^2\rangle - \langle E\rangle^2) \tag{3}$$

and the order parameter(s), to be defined below. We also produce plots of the time series for the energy and for the order parameter(s). These are vital in the interpretation of our raw data.

A Monte Carlo simulation is, of necessity, carried out for a finite lattice. In the case of periodic structures one chooses a block of unit cells and, usually, imposes periodic boundary conditions on the block. This is of course not possible for the Penrose lattice which is aperiodic. It would be possible to choose a finite piece of the lattice, with free boundary conditions, but the boundary spins would then experience a different environment and this would seriously distort the results. We have chosen instead to use the so-called 'periodic Penrose lattices' devised by Tsunetsugu *et al* (1986). These are rhombic unit cells, containing a specific number of sites N_k, which can be periodically stacked to form a structure very like the true Penrose lattice. The Penrose matching rules are broken only at a few positions. The number of sites in the kth cell is given by

$$N_k = 4F_{2k+1} + 3F_{2k} \tag{4}$$

where the $\{F_k\}$ are Fibonacci numbers. This yields unit cells containing 11, 29, 76, 199, 521, 1364, 3571, 9349, 24 476, ... sites. As $k \to \infty$ the unit cell approaches the infinite aperiodic Penrose lattice. In the work reported here we have used the 1364 and 9349 site cells, and we believe that these are large enough to provide results representative of the infinite Penrose lattice.

To explore the possible ordered phases which our system may adopt it is necessary to identify the different types of local structure which can occur. We identify seven types of site, as shown in figure 3. These do not all occur with equal frequency. In table 1 we give the numbers of each site type for the 1364, 3571 and 9349 site cells. We also give the limiting frequency of occurrence of each site type for the infinite lattice, these being simple expressions involving the golden ratio $\tau = (1+\sqrt{5})/2$. On the basis of these site types we can define seven order parameters

$$Q_\alpha = \frac{1}{N_\alpha}\sum_{i\subset\alpha}\sigma_i \qquad \alpha = 1, 2, \ldots, 7. \tag{5}$$

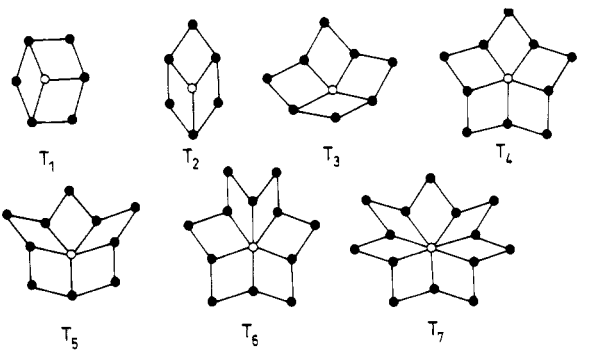

Figure 3. The seven distinct site types $T_1, \ldots, T_7$. These can be further distinguished if the larger neighbourhood is included.

Table 1. Distribution of site types in periodic Penrose lattices with $N = 1364$, 3571 and 9349 sites. The limiting frequency of occurrence of each site type in the infinite Penrose lattice is also given, in terms of the golden ratio $\tau = (1+\sqrt{5})/2$.

Site type	1	2	3	4	5	6	7
$N = 1364$	199	519	127	76	320	47	76
$N = 3571$	521	1363	324	199	841	125	198
$N = 9349$	1364	3571	843	521	2205	326	519
$N = \infty$	τ^{-4}	τ^{-2}	τ^{-5}	τ^{-6}	τ^{-3}	τ^{-7}	τ^{-6}
	0.1459	0.3820	0.0902	0.0557	0.2361	0.0344	0.0557

It may also be necessary to distinguish between sublattices; then we may consider the quantities $Q_\alpha^{A,B}$.

3. Results and discussion

We have carried out extensive Monte Carlo runs for various ratios of J'/J. On the basis of our results we are led to identify four separate regions:

(*a*) $J'/J < 1.5$ where the ordered phase is antiferromagnetic (AF);

(b) $J'/J = 1.5$, where the ordered phase is partially disordered antiferromagnetic (PDAF);

(*c*) $1.5 < J'/J < 2.0$, where the ordered phase is a more complex structure which we refer to as a partially reversed antiferromagnet (PRAF);

(*d*) $J'/J > 2.0$, where the ordered phase appears to be of a partially disordered ferrimagnetic character (PDFIM).

Our first runs were for the region $J'/J < 1.5$. As the system is cooled, from an initial disordered state, it clearly undergoes a second-order transition to an antiferromagnetic phase in which spins on the two distinct sublattices order in opposite direction. We show the ground state for the antiferromagnetic phase in figure 4. The behaviour is reversed when the temperature is slowly increased from an initial ordered state. There are no observed hysteresis effects. At $J'/J = 0$ the transition temperature is estimated to be $T_c \simeq 2.4$, in agreement with the result of Bhattacharjee *et al* (1987) for the ferromagnetic case. In figure 5 we show the observed variation of the specific heat and

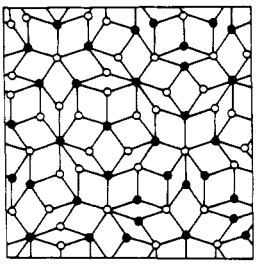

Figure 4. The antiferromagnetic state (AF) which is the ground state for $J'/J < 1.5$. Note that all of the J' bonds are frustrated.

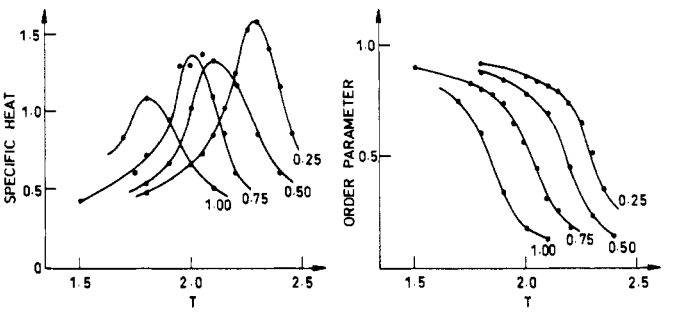

Figure 5. Temperature dependence of specific heat and antiferromagnetic order parameter, for the 1364 site cell, for various ratios of J'/J as indicated.

of the antiferromagnetic order parameter with temperature for various ratios J'/J. It should be noted that as J'/J increases the specific heat peak, giving an approximate estimate of T_c, moves to lower temperatures. Furthermore the peak decreases in height and broadens significantly as J'/J increases. This behaviour is due to an increasing degree of frustration in the system. These results shown in figure 5 are for the 1364 site cell. We have also carried out runs for larger cells. As expected the specific heat peak and order parameter variation sharpen with increasing N but there are no other qualitative differences.

As the ratio J'/J approaches 1.5 the type 2 sites become increasingly decoupled from the rest of the lattice, and at $J'/J = 1.5$ are completely free provided that the remaining sites maintain an antiferromagnetic order. We refer to this phase, shown in figure 6(a), as a partially disordered antiferromagnetic phase (PDAF). This behaviour is borne out in the Monte Carlo simulation. In figure 7 we show the time-series for the order parameters Q_1^A and Q_2^A, corresponding to type 1 and type 2 sites on sublattice A, for two temperatures, one slightly above the transition and one well below the transition. It is clear that the type 1 sites order at low temperatures (as do sites of all other types except type 2), and the order is antiferromagnetic. The type 2 sites remain disordered at all temperatures, and the fluctuations in Q_2 are independent of temperature, as shown in figure 7. The transition at $J'/J = 1.5$ occurs at $T_c \simeq 1.45$ and appears to be second order.

As J'/J increases beyond 1.5 a new type of order develops at low temperatures. The type 2 sites which were disordered at $J'/J = 1.5$ now order antiferromagnetically with their type 1 neighbours. This leads to an overall ordered phase in which the

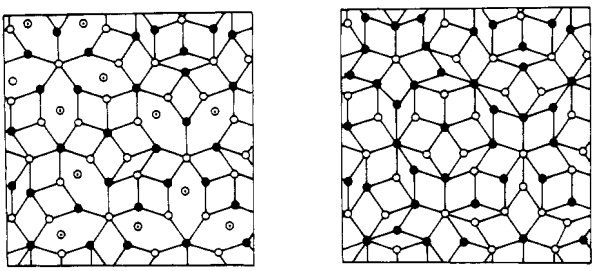

Figure 6. (*a*) The partially disordered antiferromagnetic state (PDAF) which occurs for $J'/J = 1.5$. All sites of type 2, shown as ⊙, remain disordered at all temperatures while other sites order antiferromagnetically. (*b*) The partially-reversed antiferromagnetic state (PRAF) which occurs for $1.5 < J'/J \leq 2.0$.

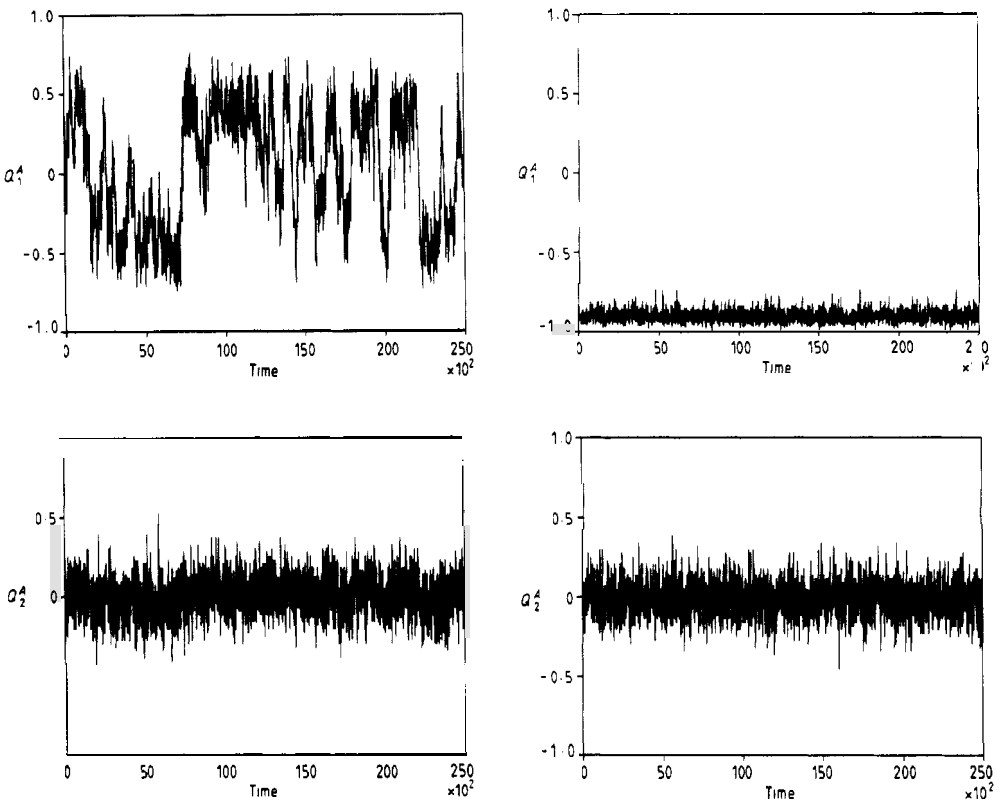

Figure 7. Time-series for Q_1^A and Q_2^A, the order parameters for type 1 and type 2 sites on sublattice *A*, for temperatures $T = 1.50$ (left) and $T = 1.00$ (right) at $J'/J = 1.5$.

antiferromagnetic ordering of site types 1, 3, 4, 5, 6, 7 remains as before with spins up on sublattice *A* and down on sublattice *B*, while type 2 sites are down on sublattice *A* and up on sublattice *B*. We refer to this phase, shown in figure 6(*b*), as a 'partially reversed antiferromagnetic' (PRAF) phase. Note that some of the *J* bonds are now frustrated. This phase appears to extend to about $J'/J = 2.0$.

Finally we turn to the region $J'/J > 2.0$. The nature of the ordered phase in this region is not immediately obvious. For $J' \gg J$ the dominant interaction will favour dimers, with opposite spin at the two sites, and trimers with the central spin opposite to the end spins, as shown in figure 8(a). If $J = 0$ then these dimers and trimers are not connected and therefore no state with long-range order will exist. For $J \neq 0$ links between the dimers and trimers may result in an ordered phase. We believe that this is indeed the case, and the ordered phase has the form shown in figure 8(b). By inspection we find that in this phase all type 1 sites are up, all sites of types 2, 3, 7 are down. Some type 4 and type 6 sites are down,, and others indeterminate, while some type 5 sites are up and others indeterminate. We refer to this phase as a partially disordered ferrimagnetic phase (PDFIM). The nature of the degeneracy which results in type 4 and 5 sites being partially disordered at all temperatures is shown in figure 8(c).

We have looked in detail at three cases, with $J'/J = 5.0$, 3.5 and 2.0. For $J'/J = 5.0$ and 3.5 the qualitative behaviour is similar. There is evidence for an ordered phase, of the type described above, at low temperatures. There appears to be a single phase transition to a high-temperature disordered phase, accompanied by a somewhat broad peak in the specific heat. However the nature of the energy fluctuations near the transition temperature is quite erratic, with significant long-time instability, and it is difficult to determine the values of the specific heat accurately. In figure 9 we show the energy time-series for $J'/J = 5.0$ and $N = 9349$, for a run of 2×10^5 sweeps. Clearly an estimate of C from (3) will be liable to error if the regions near $t = 1.3 \times 10^5$ or 1.85×10^5 are included. It may be that the behaviour of the energy, in figure 9, is indicative of two co-existing phases and a first-order transition. We are inclined to the

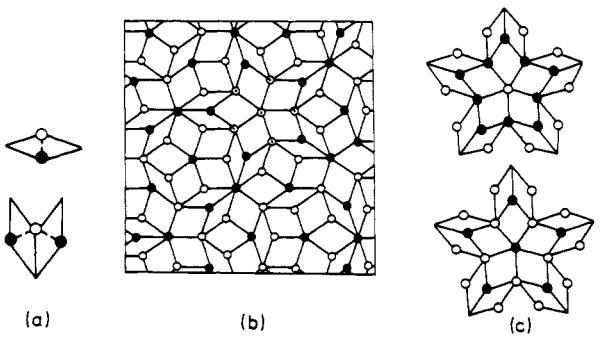

Figure 8. (a) Dimer and trimer configurations, energetically favoured for $J' \gg J$. (b) The ordered state for $J' \gg J$ (the spins shown ⊙ are indeterminate). (c) Degenerate configurations involving sites of types 4,5.

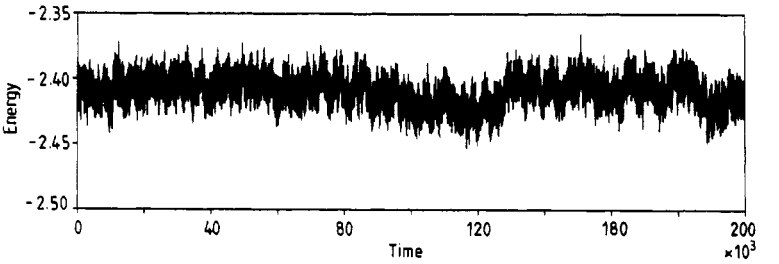

Figure 9. Energy time-series for $N = 9349$ and $J'/J = 5.0$ at temperature $T = 1.55$.

view that it is due to the existence of a large number of local minimum energy configurations and consequent non-equilibrium excursions, reminiscent of the behaviour in spin-glasses. Our prediction above, of the ordered PDFIM phase, is borne out by the data shown in figure 10. In this figure we show the evolution of the order parameters for the seven site types, Q_1 to Q_7, for $N = 9349$ and $J'/J = 5.0$. Each plot is for a total of 2×10^5 sweeps starting from a 'high' temperature $T = 1.80$ and slowly cooling through $T = 1.60$, 1.55, 1.50, 1.45, 1.40 to $T = 1.20$. As the system is cooled through the transition (around $T = 1.50$) each order parameter evolves to a non-zero value, with $Q_1 \simeq 1.0$, $Q_2 \simeq Q_3 \simeq Q_7 \simeq 1.0$ $Q_4 \simeq 0.7$, $Q_5 \simeq -0.3$ and $Q_6 \simeq 0.6$.

In figure 11 we show the specific heat for $N = 9349$ as a function of temperature, for $J'/J = 5.0$, 3.5, 2.0. In each case there is a broad peak, which we believe corresponds to a phase transition between disordered and PDFIM phases. There is considerable uncertainty in the precise values of C near the peak, as discussed above. The ratio

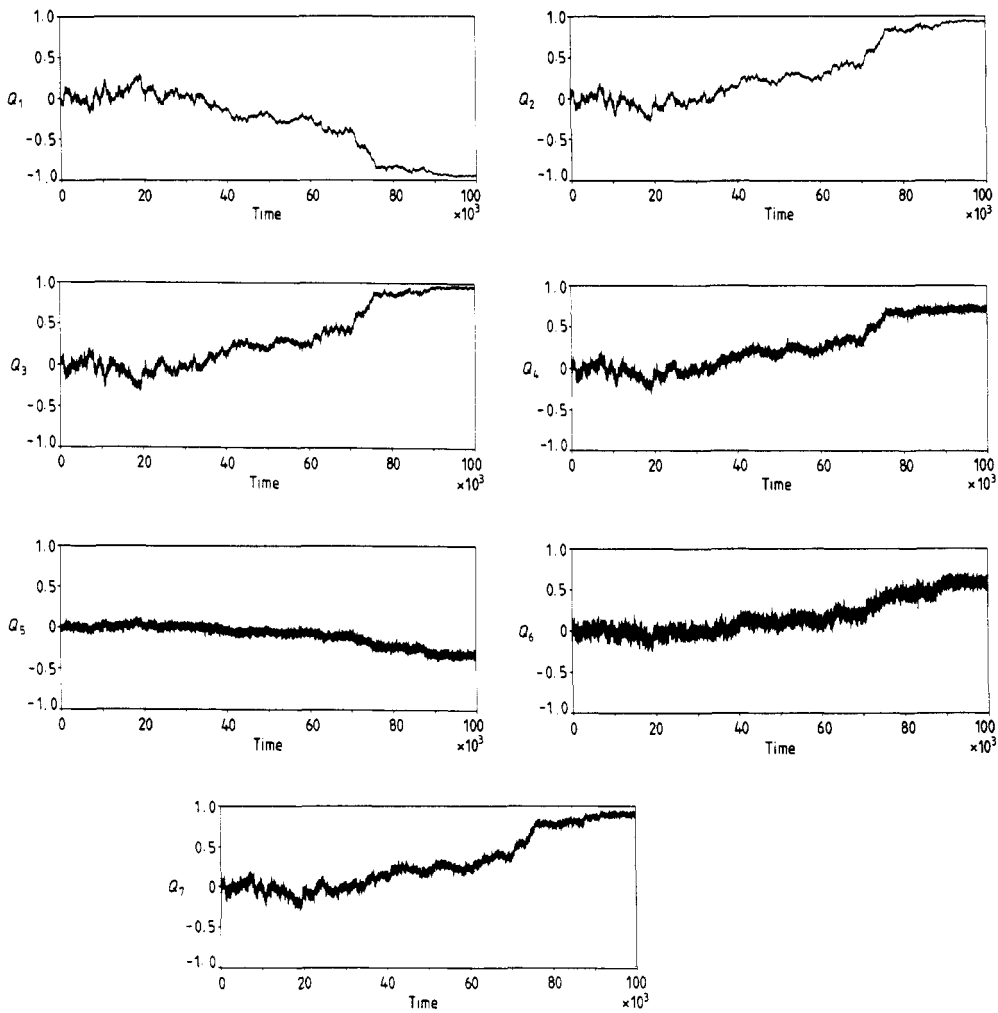

Figure 10. Order parameters $Q_1, \ldots, Q_7$ for $N = 9349$ and $J'/J = 5.0$. The temperature is initially $T = 1.80$ and the system is slowly cooled through a sequence of intermediate temperature to a final temperature $T = 1.20$.

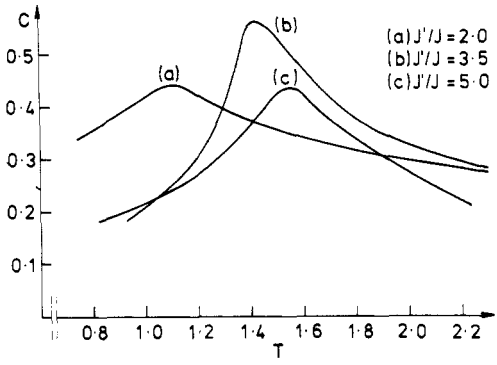

Figure 11. Specific heat for $N = 9349$ as a function of temperature, for $J'/J = 2.0, 3.5, 5.0$.

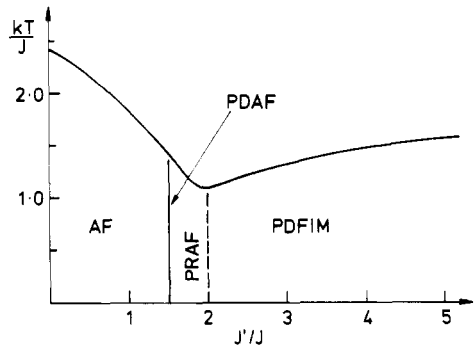

Figure 12. Predicted phase diagram for the model, showing the antiferromagnetic (AF), partially disordered antiferromagnetic (PDAF) partially reversed antiferromagnetic (PRAF) and partially disordered ferrimagnetic (PDFIM) phases. The solid and dashed lines are believed to be second- and first-order phase transition lines respectively.

$J'/J = 2.0$ lies at, or very close, to the boundary between PDFIM and PRAF phases. We have tried to locate this boundary more precisely by carrying out Monte Carlo runs at fixed temperature ($T = 0.6$) while varying J'/J slowly from 1.8 to 2.2. Large hysteresis effects are observed on crossing this, presumably, first-order line.

Our studies thus reveal a rather complex phase diagram, shown in figure 12, with at least four distinct types of ordered phase.

4. Conclusions

We have carried out extensive Monte Carlo simulations on the Ising model defined on the two-dimensional Penrose lattice with two types of antiferromagnetic interaction. For our simulations we have used large unit cells ('periodic Penrose lattices') with periodic boundary conditions, most of our results being for a cell with 9349 sites. In the limit these periodic cells tend to the infinite aperiodic Penrose lattice and we believe that our cell is large enough to avoid spurious small-lattice effects. The presence of competing interactions in our model results in subtle frustration effects. We have identified a rather complex phase diagram with four types of ordered phases: antiferromagnetic (AF), partially-disordered antiferromagnetic (PDAF), partially-reversed antiferromagnetic (PRAF) and partially-disordered ferrimagnetic (PDFIM). We believe that

these are true equilibrium phases and that the transition from each of these to the high-temperature disordered phase is second-order. We cannot, however, completely exclude the possibility that more complex types of ordering occur, either at $T = 0$ or at finite T, for some regions of J'/J or indeed that no true long-range order occurs in some regions. Certainly the very broad specific heat peak and the erratic energy fluctuations we have observed are warning signs. These features, and the very long relaxation times, are reminiscent of the behaviour of spin-glasses, with which we believe the model we have studied here shares common aspects. Further work is planned, using larger cells and also including an external magnetic field.

Acknowledgments

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