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A Monte Carlo analysis of the two-dimensional modified step model

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Abstract. The two-dimensional modified step model with nearest-neighbour interaction $C(\theta)=0$ for $|\theta|\leqslant\delta\pi$, $C(\theta)=1$ for $\delta\pi<|\theta|<\pi$ and $C(\theta+2\pi)=C(\theta)$ is studied by Monte Carlo simulation. Using Migdal transformations Barber found evidence of a phase transition for this model for $0.05\leqslant\delta\leqslant 0.43$. We have studied the model for $\delta=0.1$ and $\delta=0.25$ on a number of finite lattices and also find evidence of a phase transition, with critical temperature $T_c\approx 1.25$ and $T_c\approx 1.5$ respectively.

1. Introduction

In recent years the critical behaviour of two-dimensional planar lattice spin systems has attracted considerable interest. We can define the Hamiltonian for this general class of model by

$$H=-\sum_{\langle ij\rangle}\sum_{\alpha=1}^{N}J_\alpha S_i^{(\alpha)}S_j^{(\alpha)} \tag{1.1}$$

where $(J_1,\ldots,J_N)$ and $(S_i^{(1)},\ldots,S_i^{(N)})$ are N-dimensional interaction and spin vectors respectively and the summation is over nearest-neighbour lattice sites $\langle ij\rangle$. $\mathbf{J}$ is an N-dimensional second-order diagonal tensor, but we use the conventional notational simplification of treating it as an N-dimensional vector. For $N=2$ we can associate an angle θ_i and interaction function $C(\theta_i)$ with each vector $\boldsymbol{S}_i$ and can write

$$H=-J\sum_{\langle ij\rangle}C(\theta_i-\theta_j) \tag{1.2}$$

where now $J=J_1=J_2$ corresponding to the isotropic case.

The planar model is defined by

$$C(\theta)=1-\cos(\theta) \tag{1.3}$$

and the step model by

$$C(\theta)=\begin{cases}0 & |\theta|\leqslant\pi/2\\ 1 & \pi/2<|\theta|<\pi\end{cases} \tag{1.4}$$
$$C(\theta+2\pi)=C(\theta).$$

Domany *et al* (1984) defined the modified planar model by

$$C(\theta)=1-[\cos^2(\theta/2)]^{p^2} \tag{1.5}$$

and Barber (1983) defined the modified step model by

$$C(\theta)=\begin{cases}0 & |\theta|\leqslant\delta\pi\\ 1 & \delta\pi<|\theta|<\pi\end{cases} \tag{1.6}$$
$$C(\theta+2\pi)=C(\theta).$$

For $p=1$, (1.5) reduces to the planar model interaction function, and for $\delta=\frac{1}{2}$,

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(1.6) reduces to the step model interaction function. These functions are all shown in figure 1.

The Monte Carlo method has gained increased popularity over recent years. Very recent work by Berretti and Sokal (1986) has called for greater statistical rigour to be used in Monte Carlo studies. Monte Carlo analyses of the planar model have been carried out by Miyashita *et al* (1978), Tobochnik and Chester (1979), Fucito (1983) and Fucito and Solomon (1984), and of the step model by Nymeyer and Irving (1986). The modified planar model has been studied by Domany *et al* (1984) and Van Himbergen (1984), also using the Monte Carlo technique, while the modified step model has been analysed by Barber (1983) using a Migdal renormalisation group scheme.

While the step and planar models have apparently similar underlying symmetries, their behaviour in two dimensions appears to be radically different. From Mermin and Wagner (1966) we know that the planar model cannot undergo a conventional phase transition. Work by Kosterlitz and Thouless (1973) has shown that the planar model instead undergoes an unconventional phase transition. This transition occurs when the bound vortex-antivortex pairs which populate the low temperature phase begin to unbind. The low temperature phase is said to have topological long range order.

The proof by Mermin and Wagner does not apply to the step model due to the discontinuous interaction function. The step model does not have a topologically induced phase transition. This is intuitively obvious (vortices do not provide any energy advantage) and has been shown by series analysis (Guttmann 1978, Nymeyer and Guttmann 1985). Other series analyses (Guttmann and Joyce 1973, Guttmann and Nymeyer 1978) have not found any evidence for a conventional (or unconventional) phase transition. Barber (1983) also finds no evidence of a phase transition for the step model.

Recent Monte Carlo work by Domany *et al* (1984) and Van Himbergen (1984) have shown that quite dramatic changes in behaviour may occur for the modified planar model. The continuous phase transition of the planar model ($p = 1$) changes into a first-order transition as p increases. Van Himbergen suggests that the narrowness of the well (corresponding to large p) is instrumental in this change of behaviour. A narrow well inhibits the formation of vortex-antivortex pairs at low temperature. If p is large enough, as the critical temperature is approached large number of vortices will be formed very suddenly, and lead to a first-order transition. The critical value of p appears to be 3.

This paper follows an earlier paper (Nymeyer and Irving 1986, hereafter referred to as I) in which we studied the step and planar models using the Monte Carlo technique. In I we found evidence to suggest that there is no phase transition for the step model. In this paper we carry out a similar analysis on the modified step model to determine the effect of a narrow well in the interaction function on the thermodynamic behaviour. Increasing p in the case of the modified planar model and decreasing δ in the case of the modified step model reduces the size of the well in the interaction function (see figure 1).

Barber (1983) first studied the modified step model. He applied a Migdal transformation to a number of planar spin systems on a number of regular planar lattices. At a given temperature, repeated applications (iterations) of the transformation can result in a 'fixed point'. In the planar model the low temperature region is populated by an infinite number of 'fixed points' corresponding to a line of critical points. In the step model all temperatures iterate to the infinite-temperature 'fixed line'. The step model

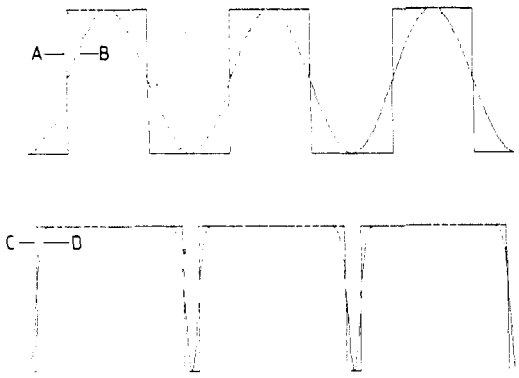

Figure 1. The interaction functions of the A, step model; B, planar model; C, $\delta = 0.1$ modified step model and D, $p = 6$ modified planar model.

is therefore 'stuck' in the disordered phase. In the modified step model, on the other hand, there is evidence of a 'fixed line' for $0.05 \leqslant \delta \leqslant 0.43$, and so for these values of δ the modified step model should undergo a phase transition.

Our aim in this paper is to confirm Barber's results by studying the modified step model with $\delta < \frac{1}{2}$ and comparing with the step model ($\delta = \frac{1}{2}$). In particular we analyse the $\delta = 0.1$ and $\delta = 0.25$ (modified step) models. To check the equilibration time of the system and the independence of the data we have carried out an autocorrelation analysis as part of our Monte Carlo analysis.

2. Results

The Metropolis Monte Carlo scheme we have used is similar to the scheme outlined in Tobochnik and Chester (1979).

For a given box size ($n \times n$), we use a hot start (all spins pointing in a random direction) at $T = 3.0$, and equilibrate the system with either 1000 or 5000 sweeps through the lattice. We then carry out a further 2000 sweeps, which are broken up into 10 blocks of 200 sweeps. Each of the calculated thermodynamic variables are averaged over each block of spins, and then averaged again over the 10 blocks. This provides one data point, which is considered to be independent. The temperature is decremented and the process repeated using the last configuration at the previous (higher) temperature as the starting configuration. When the lowest temperature is reached ($T = 0.25$), we have completed the cooling cycle, and have one data point for each temperature. We then repeat the process in the reverse direction, increasing the temperature at each step, until the highest temperature is again reached. This gives us a second data point at each temperature. The two data points are averaged. Subaverages are checked for drift (i.e. any monotonic movements) and for consistency.

For each of the three models (i.e. the $\delta = 0.5$, $\delta = 0.25$ and $\delta = 0.1$ models) we have carried out the above procedure on the 8×8, 16×16, 32×32, 64×64 and 100×100 spin lattices. For each lattice, averages were calculated at 21 temperatures between $T = 0.25$ and $T = 3.0$.

The thermodynamic quantities that we studied are the energy per spin, specific heat, mean square angular displacement, correlation function and susceptibility. As

in I we define these by

$$\begin{aligned} &\text{energy:} && \langle E\rangle = N^{-1}\langle H\rangle \\ &\text{specific heat:} && C_v = \beta^2 N^{-1}(\langle E^2\rangle - \langle E\rangle^2) \\ &\text{correlation function:} && C(r) = \langle \cos(\theta_r - \theta_0)\rangle \\ &\text{susceptibility:} && \chi = \sum_{i=1}^{n} C(i) \end{aligned} \tag{2.1}$$

where the lattice is of size $n \times n = N$ and $T = 1/\beta J$. The mean-square angular displacement $\langle \theta^2 \rangle$ is calculated by subtracting from each angle θ_i the average spin direction.

The behaviour of the above functions for the (isotropic) $\delta = 0.5$ model was studied in detail in I. Corresponding results for the $\delta = 0.1$ and $\delta = 0.25$ models will be described in this paper.

It is a simple calculation to show that in the infinite temperature limit the average energy per spin for the modified step model is $2(1-2\delta)$. This is consistent with the behaviour shown in figure 2 where we plot $\langle E\rangle/N$ for the $\delta = 0.5$, 0.25 and 0.1 models on the 64×64 lattice.

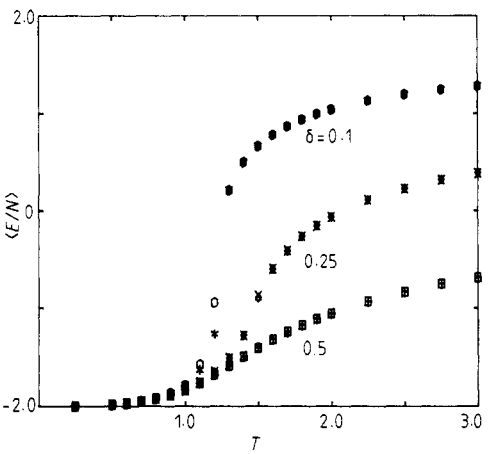

Figure 2. Plot of energy per spin against temperature. □(+), ◇(×) and ◯(*) correspond to the cooling (heating) cycle for the $\delta = 0.5$, $\delta = 0.25$ and $\delta = 0.1$ models (respectively) on the 64×64 lattice.

Notice that there is a large discrepancy between the heating and cooling data at $T = 1.2$ ($\delta = 0.1$ model) and a somewhat smaller discrepancy at $T = 1.5$ ($\delta = 0.25$ model). It has proved difficult to determine the cause of these discrepancies due to the steep slope of the energy curves and the unstable behaviour of the models of these temperatures. To overcome these problems very long runs (up to 4×10^5 sweeps) were carried out using different starting conditions. No clear picture emerged however. The energy jumped between high and low temperature values erratically, particularly on the smaller lattices. On the larger lattices it was not possible to use enough sweeps to reduce the size of the confidence intervals sufficiently.

Note that none of these behavioural problems occurred with the $\delta = 0.5$ model (see I), where the energy data were found to be well behaved and showed no signs of 'discrepancies' or hysteresis.

In figure 3 we plot the behaviour of the specific heat for each of the three models. Two sets of data are shown. The curve joins data points which are averages of the heating and cooling data for all the lattices. The extra data points, the crosses and open squares, correspond to longer runs at the 'peaking' temperatures on the 16×16 and 32×32 lattices respectively. Each of these extra data points is an average over 2000 sweeps of the lattice. Between each block of 2000 sweeps, 8000 sweeps were carried out to ensure independence of the data. For comparison purposes we also carried out an extra run at $T=1.1$.

We estimate that the peaks occur at $T=1.25$ for the $\delta=0.1$ model, and $T=1.5$ for the $\delta=0.25$ model, while for $\delta=0.5$ there is no apparent peaking (see figure 2 in I).

Following Tobochnik and Chester (1979), we studied the mean-square angular displacement $\langle\theta^2\rangle$, shown in figure 4(*a*) ($\delta=0.25$ model), figure 4(*b*) ($\delta=0.1$ model) and figure 4(*c*) ($\delta=0.5$ model).

If we integrate θ^2 over all minimum energy configurations (low temperature) we find

$$I_{\mathrm{LT}}(\theta^2)=\frac{1}{2\delta\pi}\int_{-\delta\pi}^{\delta\pi}\theta^2\,\mathrm{d}\theta\approx\begin{cases}0.822 & \delta=0.5\\ 0.206 & \delta=0.25\\ 0.033 & \delta=0.1\ .\end{cases}\tag{2.2}$$

At high temperature, where spins are pointing in random directions, we have

$$I_{\mathrm{HT}}(\theta^2)=\pi^2/3\approx3.29.\tag{2.3}$$

This behaviour is consistent with that shown in figures 4(*a*) and 4(*b*). Note the differences in behaviour between the $\delta=0.25$ and $\delta=0.1$ models shown in figures 4(*a*) and 4(*b*) and the $\delta=0.5$ model shown in figure 4(*c*). The jump in $\langle\theta^2\rangle$ is much sharper, and the lattice contours are rapidly converging to $T\approx1.25$ ($\delta=0.1$ model) and $T\approx1.5$ ($\delta=0.25$ model).

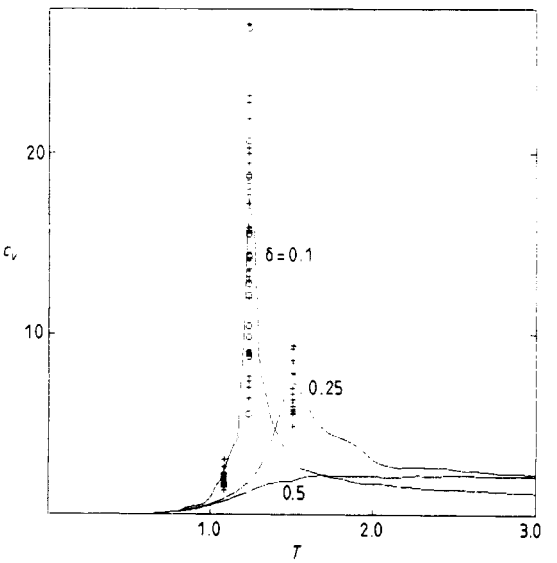

Figure 3. Plot of the specific heat against temperature for the $\delta=0.5$, $\delta=0.25$ and $\delta=0.1$ models. The dots are averages over all lattices and are joined by a curve as a guide. The crosses and open squares are further averages taken using the 16×16 and 32×32 lattices (respectively).

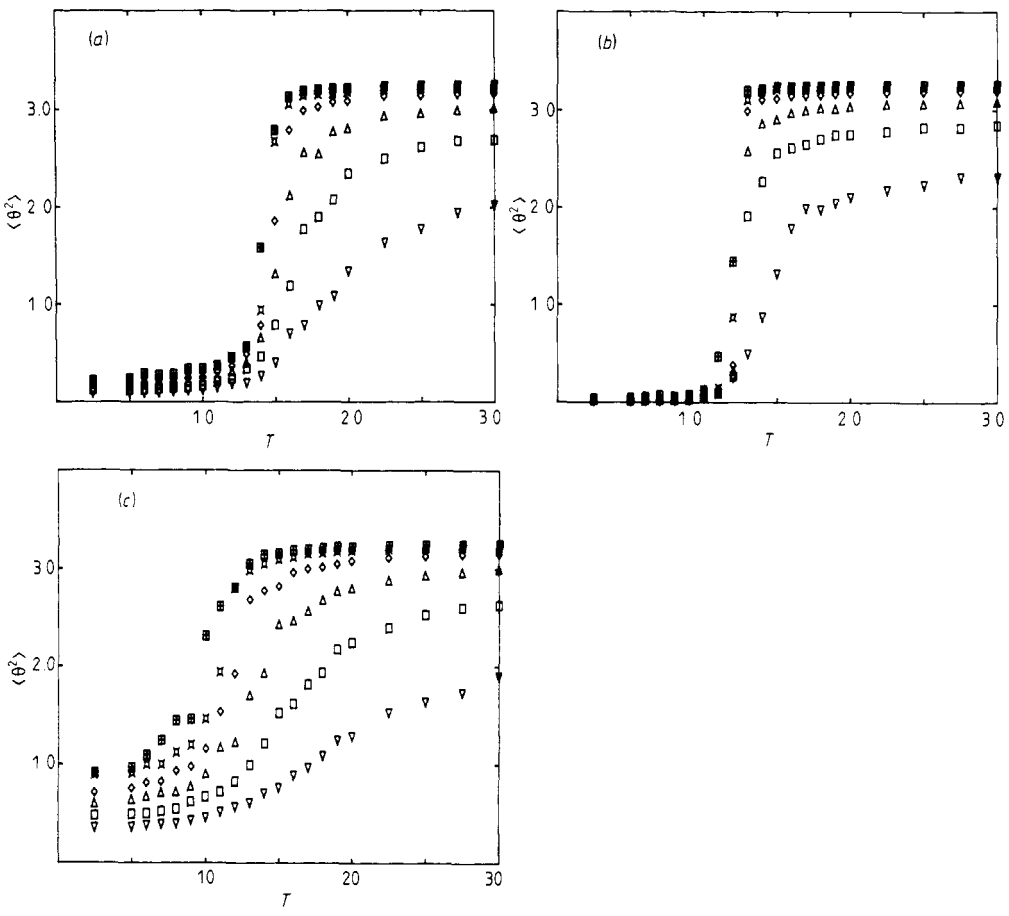

Figure 4. Plot of $\langle\theta^2\rangle$ against temperature for (a) the $\delta = 0.25$ model, (b) $\delta = 0.1$ model and (c) $\delta = 0.5$ model on the 4×4 (▽), 8×8 (□), 16×16 (△), 32×32 (◇), 64×64 (⊡) and 100×100 (⊠) lattices.

The behaviour of $C(n/2)$ is shown in figures 5(a) and 5(b) for the $\delta = 0.25$ and $\delta = 0.1$ models respectively. Since $n \times n = N$ is the lattice size, $n/2$ is the maximum effective distance we can calculate the correlation function.

We can again approximate the low temperature behaviour by integrating over the well in the interaction function, i.e.

$$I_{\mathrm{LT}}(\cos(\theta)) = \frac{1}{2\delta\pi}\int_{-\delta\pi}^{\delta\pi}\cos(\theta)\,\mathrm{d}\theta \approx \begin{cases} 0.637 & \delta = 0.5 \\ 0.900 & \delta = 0.25 \\ 0.984 & \delta = 0.1 \end{cases} \tag{2.4}$$

and of course at high temperature we have that

$$I_{\mathrm{HT}}(\cos(\theta)) = 0. \tag{2.5}$$

Again there is a striking difference between the behaviour of the $\delta = 0.1$ and $\delta = 0.25$ models (figures 5(a) and 5(b)) and the $\delta = 0.5$ model (figure 4 in I). We argued in I that the behaviour of the correlation function in a finite system can provide evidence of a phase transition in an infinite system. $C(n/2)$ will have 'step function'-like

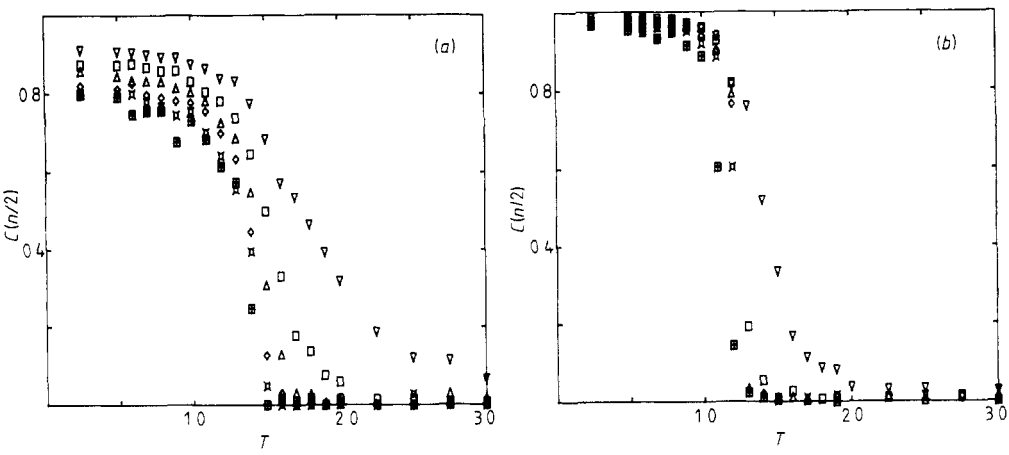

Figure 5. Plot of the correlation function against temperature for spins $n/2$ sites apart for the (a) $\delta = 0.25$ model and the (b) $\delta = 0.1$ model on the 4×4 (∇), 8×8 ($\square$), 16×16 ($\triangle$), 32×32 ($\diamond$), 64×64 ($\square$) and 100×100 ($\boxtimes$) lattices.

behaviour centred on a pseudo-critical point $T_{c,n}$. If there is a phase transition, as n increases the underlying 'step function' will become sharper, and $T_{c,n}$ will converge to the 'real' critical temperature T_c.

This is precisely the behaviour we can see in figures 5(a) and 5(b), and the critical temperatures $T \approx 1.25$ ($\delta = 0.1$ model) and $T \approx 1.5$ ($\delta = 0.25$ model) are indicated. This contrasts with the behaviour shown in figure 4 in I ($\delta = 0.5$ model).

In figure 6 we plot the behaviour of the susceptibility for the $\delta = 0.1$ and $\delta = 0.5$ models. The sharp increase in χ for the $\delta = 0.1$ model occurs at $T \approx 1.25$.

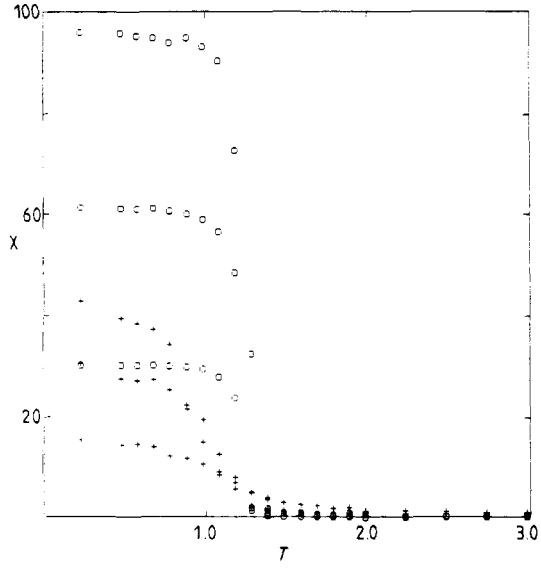

Figure 6. Plot of the susceptibility against temperature of the $\delta = 0.5$ model (crosses) and $\delta = 0.1$ model (open squares) on the 32×32, 64×64 and 100×100 lattices (in ascending order).

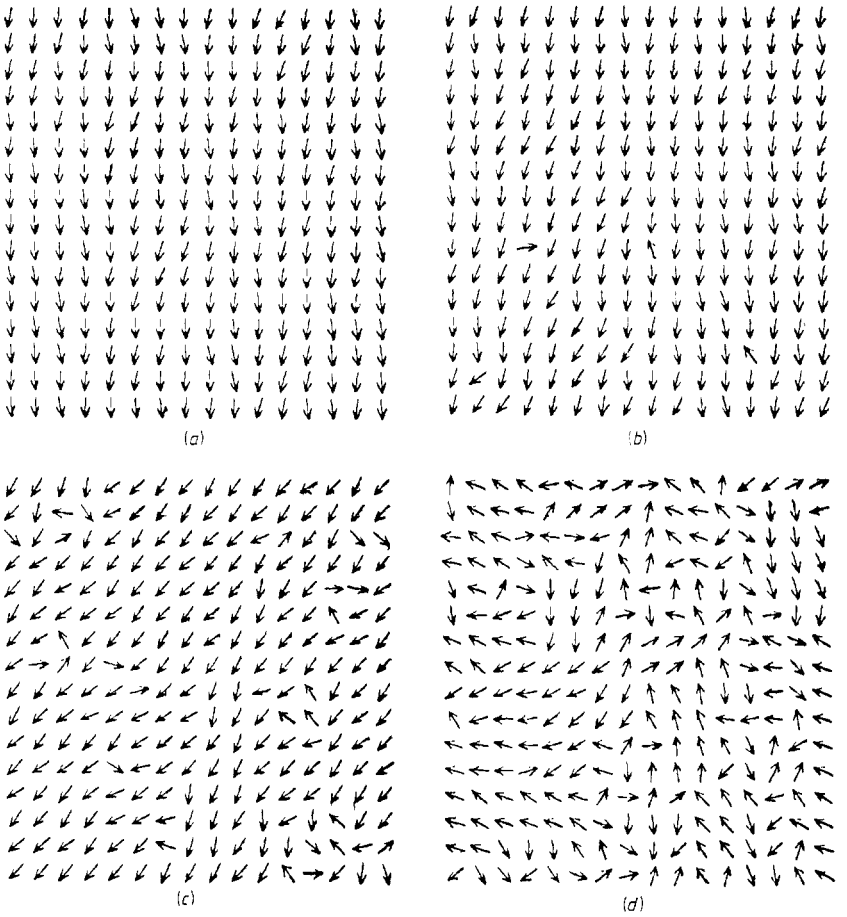

Figure 7. Typical (16×16) spin configurations for the $\delta = 0.1$ model at (a) $T = 0.25$, (b) $T = 1.1$, (c) $T = 1.2$ and (d) $T = 1.3$.

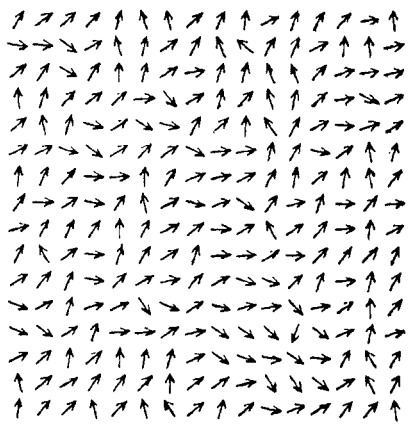

Figure 8. Typical (16×16) spin configuration for the $\delta = 0.5$ model at $T = 0.25$.

In figures 7(*a*)-7(*d*) we show typical spin configurations for the $\delta = 0.1$ model at $T = 0.25$, 1.1, 1.2 and 1.3 respectively. In figure 8 we show the $\delta = 0.5$ model at $T = 0.25$ only. At each of these temperatures the lattice was hot started and allowed to equilibrate over 4000 sweeps. A cold start showed the same behaviour, as did varying the lattice size.

While the $\delta = 0.5$ model (figure 8) appears to be disordered at even its 'lowest' temperature, the $\delta = 0.1$ model shows a remarkable degree of alignment for $T \leqslant 1.2$. Above this temperature the system appears to be disordered. For the $\delta = 0.25$ model the spins are ordered for $T \leqslant 1.5$, and disordered above. So, while the $\delta = 0.1$ and $\delta = 0.25$ models appear to have an ordered low temperature phase, the $\delta = 0.5$ model apparently has only a single disordered phase.

A time series analysis was also carried out on the data. The procedure is the same as that outlined in I, and uses the expression

$$F(t) = \frac{1}{l-t} \sum_{i=1}^{l-t} (x_i - \bar{x})(x_{i+t} - \bar{x}_{i+t})/S_i S_{i+t} \tag{2.6}$$

where l is the run length, $t \in [0, l-1]$ and x is the sample data with

$$\begin{aligned} \bar{x}_i &= \sum_{i=1}^{l-t} x_i/(l-t) \\ \bar{x}_{i+t} &= \sum_{j=t+1}^{l} x_j/(l-t) \\ S_k &= (\overline{x_k^2} - \bar{x}_k^2)^{1/2}. \end{aligned} \tag{2.7}$$

The aim of this analysis is to measure the independence of the data. This is necessary if meaningful statistical averages and errors are to be calculated. This analysis was only carried out on the 16×16 and 32×32 lattices. The results for the $\delta = 0.5$ model are outlined in I. Only the $\delta = 0.1$ model behaviour will be described here.

The autocorrelation time t_a is the shortest time $t = t_a$ such that $F(t_a) \leqslant 0.1$. In practice it is necessary to use a run length $l \gg t_a$ otherwise 'noise' will swamp the behaviour of $F(t)$.

A small value of t_a, and small frequently oscillating behaviour for $F(t)$, suggests the data are essentially uncorrelated. We expect this type of behaviour at high temperature. A large value of t_a means the data are correlated and can be the result of critical 'slowing down'.

The procedure used was first to generate all the data points. These data points are the energy and magnetisation after each sweep of the lattice. From these data all the required thermodynamic functions can be calculated. At each temperature the energy data were analysed using (2.6), and values of l of 2000 and 4000.

The resulting function at temperatures $T = 0.5$, 1.25 and 2.5 for $t < 200$ is plotted in figure 9. In general, at low and high temperature the behaviour of $F(t)$ was fairly consistent. Near criticality, at $T = 1.2$ and $T = 1.3$ there was some erratic behaviour, and at $T = 1.25$ it took a large number of sweeps for $F(t)$ to settle down. The erratic behaviour was worst for the smaller lattices. For these lattices the location of the energy jump was somewhat 'blurred', in that the system would often jump between low and high temperature energy levels. As the lattice size increased, this effect became less apparent.

From the behaviour of $F(t)$, t_a was estimated. In the low temperature region (i.e. $T < 1.2$) we found $10 \leqslant t_a \leqslant 20$, and in the high temperature region ($T > 1.3$), $2 \leqslant t_a \leqslant 10$. At $T = 1.25$ we estimated $t_a \approx 75$.

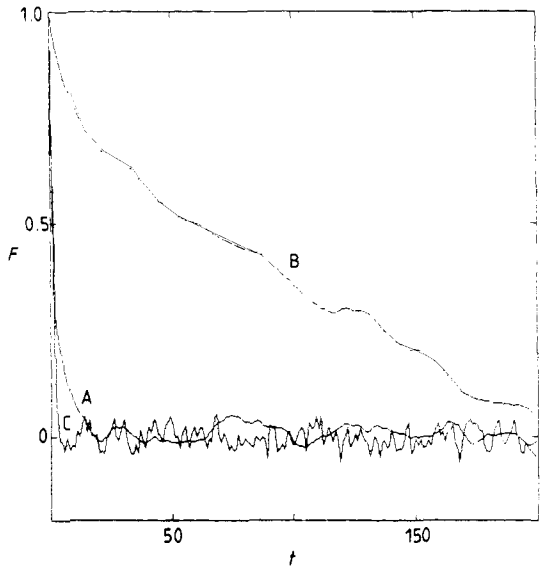

Figure 9. Typical behaviour of $F(t)$ for the energy of the $\delta = 0.1$ model at A, $T = 0.5$; B, $T = 1.25$ and C, $T = 2.5$.

Given a value for t_a we consider every t_ath energy data point to be independent, and using this we can calculate the average energy and standard errors. In table 1 we list the results for the energy at $T = 0.5$, 1.25 and 2.5. Notice the difference in the energy at $T = 1.25$ for the smaller lattices. A large number of sweeps ($\sim 8 \times 10^5$) was carried out to verify that the system was properly equilibrated.

While the energy did show a 'small n' effect, all the results obtained in the autocorrelation analysis are consistent with those given earlier.

Table 1. The energy per spin of the $\delta = 0.1$ model on various lattices.

	$T = 0.5$	$T = 1.25$	$T = 2.50$
8×8	-1.9870 ± 0.0001	-0.845 ± 0.005	1.1944 ± 0.0010
16×16	-1.9863 ± 0.0001	-0.251 ± 0.008	1.1969 ± 0.0007
32×32	-1.9863 ± 0.0001	-0.045 ± 0.003	1.1966 ± 0.0004
64×64	-1.9862 ± 0.0003	-0.048 ± 0.002	1.1965 ± 0.0002
100×100		-0.045	

3. Discussion

It appears likely that the modified step model for $\delta = 0.1$ and $\delta = 0.25$ undergoes some kind of phase transition. All the thermodynamic quantities studied show an abrupt change in behaviour at $T \approx 1.25$ ($\delta = 0.1$) and $T \approx 1.5$ ($\delta = 0.25$).

We have not been able to confirm or deny the existence of hysteresis for these models, probably because of the large temperature grid that we have used. Note, however, that no evidence for hysteresis was found for the $\delta = \frac{1}{2}$ model in I.

The specific heat is poorly behaved, but did reveal large sharp peaks at the above temperatures for the $\delta = 0.1$ and $\delta = 0.25$ models in contrast to the 'flat' behaviour of

the $\delta = \frac{1}{2}$ model. The behaviour of the correlation function suggests quite strongly that a critical point does exist for the $\delta = 0.1$ and $\delta = 0.25$ models, but not for the $\delta = \frac{1}{2}$ model. Both the mean angular displacement and the susceptibility show sharp 'step function'-like behaviour at the above temperatures.

These results confirm the results of Barber (1983). He finds that while the step model is 'stuck' in a disordered phase, the modified step model for $0.05 \leqslant \delta \leqslant 0.43$ does appear to undergo a phase transition, and estimates $T = T_c \approx 1.45$ ($\delta = 0.1$) and $T = T_c \approx 1.8$ ($\delta = 0.25$). While these estimates are slightly larger than ours they are, given the possible errors inherent in the Monte Carlo and Migdal methods, not unreasonably so.

Van Himbergen (1984) has suggested that the modified planar model undergoes a different type of transition to the ordinary planar model due to the inhibiting effect of the narrow-well interaction function on the formation of vortices at low temperature. While this mechanism is obviously not at work in the modified step model, our results are qualitatively consistent with those of Domany *et al* and Van Himbergen who find increasingly 'strong' critical behaviour as the interaction function is more highly modified.

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