A Monte Carlo analysis of the two-dimensional planar and step models

1986 J. Phys. A: Math. Gen. 19 1745

(http://iopscience.iop.org/0305-4470/19/9/046)

J. Phys. A: Math. Gen. 19 (1986) 1745-1752. Printed in Great Britain

COMMENT

A Monte Carlo analysis of the two-dimensional planar and step models

A Nymeyer† and A C Irving‡

† Department of Mathematics, Statistics and Computer Science, University of Newcastle, NSW 2308, Australia

‡ Department of Applied Mathematics and Theoretical Physics, University of Liverpool, PO Box 147, Liverpool L69 3BX, UK

Received 8 January 1985, in final form 5 August 1985

Abstract. Using the Metropolis Monte Carlo scheme we have analysed and compared the behaviour of the two-dimensional classical planar and step models. In particular, we have analysed the energy, specific heat, correlation function and susceptibility on a range of finite lattices. While both models show similar numerical difficulties, it is argued that in the case of the step model a phase transition is unlikely.

Two-dimensional models provide a surprisingly rich field of research. In 1966 Mermin and Wagner proved that no long range order (and hence no spontaneous magnetisation) could exist for certain two-dimensional models with a symmetric and continuous interaction function. In 1973 Kosterlitz and Thouless put forward a mechanism by which certain two-dimensional models could have a phase transition, but have no long range order. Models in this category have a low temperature phase occupied by bound vortex-antivortex pairs. At the critical temperature these pairs dissociate and lead to increasing disorder in the system.

One of the most frequently studied two-dimensional models is the planar classical Heisenberg model given by the Hamiltonian

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

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 pairs $\langle ij \rangle$. Strictly speaking, $\boldsymbol{J}$ is an N-dimensional, second-order diagonal tensor, but we adopt the conventional notational simplification of treating it as a N-dimensional vector.

If we restrict to $N = 2$, we can associate an angle θ_i and interaction function $C(\theta_i)$ with each vector $\boldsymbol{S}_i$ and can write

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

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

We define the planar classical Heisenberg model Hamiltonian by letting $C(\theta) = \cos(\theta)$ and the step model by $C(\theta) = 1$ for $|\theta| \leqslant \pi/2$, $C(\theta) = -1$ for $\pi/2 < |\theta| < \pi$ and $C(\theta + 2\pi) = C(\theta)$.

0305-4470/86/091745+08$02.50

The Mermin and Wagner proof excludes a conventional phase transition for the planar model. It does not, however, apply to the step model because the interaction function is discontinuous. The planar model in contrast undergoes a phase transition of the type formulated by Kosterlitz and Thouless (1973). The step model does not have a vortex induced transition since the formation of vortices is not energetically favourable. This has been confirmed by series analysis (Guttmann 1978, Nymeyer and Guttman 1985).

In this comment we study and compare the behaviour of the planar and step models with a view to understanding firstly the extent of the differences in behaviour and secondly to shed more light on the question of the existence of a phase transition for the step model. We use the traditional Metropolis Monte Carlo scheme already used extensively on the planar model (Miyashita *et al* 1978, Tobochnik and Chester 1979, Fucito 1983, Fucito and Solomon 1983) but not on the step model. Work by these authors has proved invaluable as a check on our calculations.

The theory underlying the Monte Carlo scheme has been well documented (Metropolis *et al* 1953, Valleau and Whittington 1977). In this scheme we generate a representative sample of states on a finite lattice. To obtain estimates of thermodynamic functions we simply average over these states.

The Monte Carlo procedure used is similar to that outlined in Tobochnik and Chester (1979). We have, however, increased the number of equilibrium sweeps from 1000 to 2000, and the number of sweeps used to calculate averages from 2000 to 5000, and we have used a larger number of lattices.

The heating and cooling data are collected at temperatures 0.25, 0.5 to 2.0 in steps of 0.1, 2.25, 2.50, 2.75 and 3.0. The lattice sizes we use are 8×8, 16×16, 32×32, 64×64 and 100×100. The planar model, however, was not analysed on the 100×100 lattice as the interaction function for the planar model took substantially longer to evaluate than that for the step model. Unless stated otherwise, the data points shown on the plots will be averages of the heating and cooling data.

The energy per spin and the specific heat for both models were calculated using

$$\langle E\rangle = (1/N)\langle H\rangle$$

and

$$C = \beta^2 \tilde{C} = (\beta^2/N)(\langle E^2\rangle - \langle E\rangle^2)$$

where we have already defined the Hamiltonian H, and $n\times n = N$ is the lattice size. We let T stand for $1/\beta J$.

In figure 1 we plot the energy per spin of the step and planar models, for both heating and cooling cycles. There was no evidence of hysteresis for either model. The data, however, are not accurate enough for a 'small amount' of hysteresis to be detectable. Indeed, for the smaller lattices there was some discrepancy between the heating and cooling energy data. The amount of discrepancy decreased with increasing lattice size, and was not discernible on the largest lattice of each model (shown in figure 1). Increasing the number of equilibration sweeps (from 1000 to 5000) between successive temperatures did not affect the data shown in figure 1.

In agreement with Miyashita *et al* (1978) we found the specific heat peak of the planar model to be located between $T = 1.1$ and $T = 1.15$ and this was verified by much longer runs ($\sim$100 000 sweeps) on the 16×16 and 32×32 lattices. This value is significantly higher than the estimate of Tobochnik and Chester (1979) of $kT/J = 1.02$. The specific heat of the step model is plotted in figure 2. For both models the specific heat appears to be lattice independent.

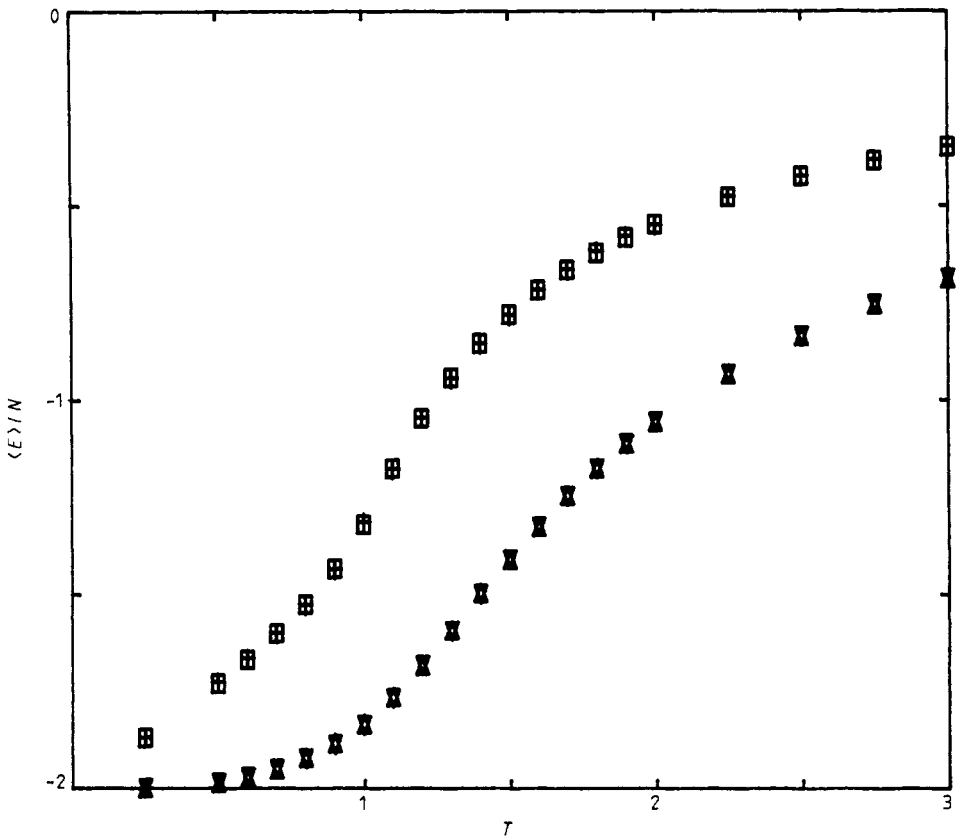

Figure 1. Plot of energy per spin against temperature. △ and ▽ correspond to the cooling and heating cycle (respectively) for the step model on the 100×100 lattice, and likewise □ and + to cooling and heating cycles for the planar model on the 64×64 lattice.

We have calculated the correlation function by two methods. Firstly we used the simple expression

$$C(j) = \langle \cos(\theta_i - \theta_{i+j}) \rangle$$

where spin $i+j$ is separated from spin i by j spins in the vertical (or horizontal) direction. The second method involves calculating the total magnetisation in the x and y directions of each column (say), $\boldsymbol{M}(j) = (M_x(j), M_y(j))$ where $j = 1$ to n. It is then a simple matter to calculate the correlation between the columns, and hence the correlation function by using

$$C(j) = \left\langle (1/n) \sum_{i=1}^{n} \boldsymbol{M}(i) \cdot \boldsymbol{M}(i+j) \right\rangle.$$

The second method extracts more information from each sweep of the lattice. Both methods, however, give the same qualitative result.

In figure 3 we plot the behaviour of $C(n/2)$ for the planar and step models respectively, where $n \times n = N$ is the lattice size. Since we use periodic boundary conditions the maximum effective distance we can calculate $C(j)$ is $n/2$. If we assume that for the step model the spins at low and high temperature are pointing randomly

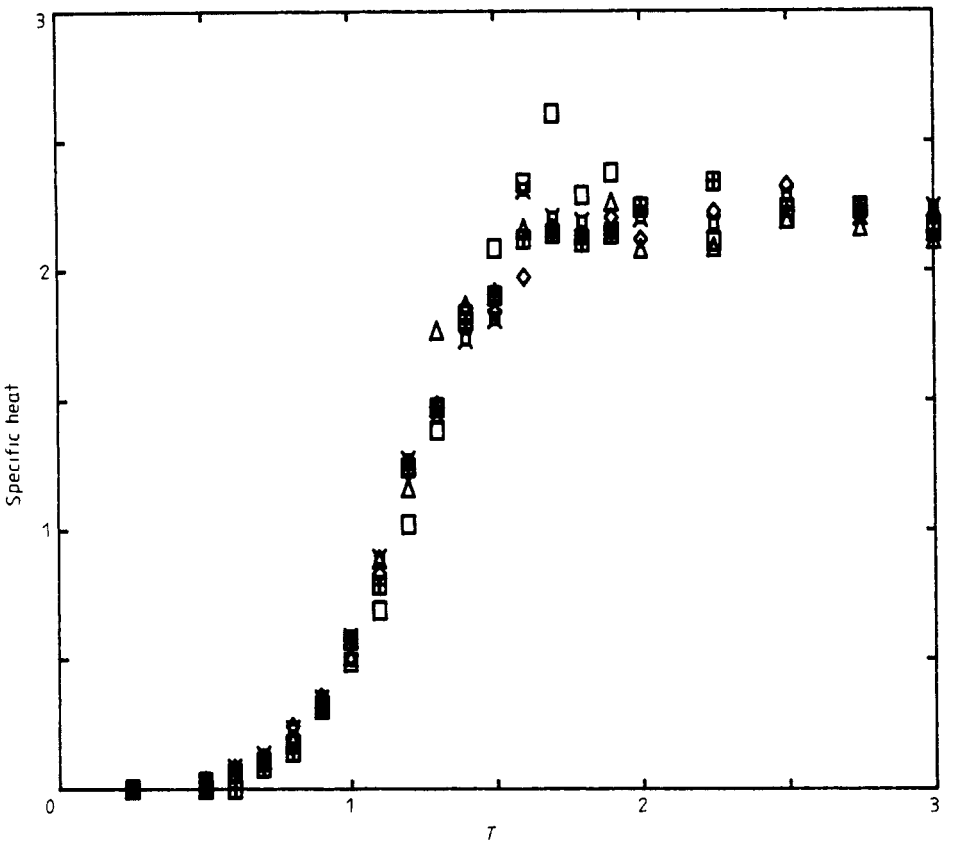

Figure 2. Plot of specific heat against temperature for the step model on the 8×8 (□), 16×16 (△), 32×32 (◇), 64×64 (¤) and 100×100 (⊠) lattices.

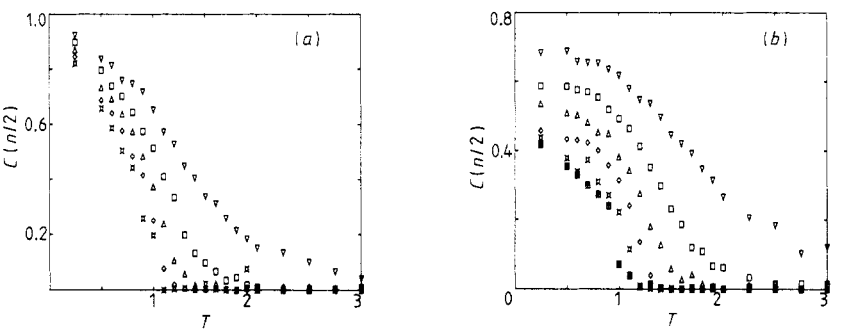

Figure 3. Plot of the correlation function against temperature for spins $n/2$ sites apart for the planar model (a) and step model (b) on the 4×4 (▽), 8×8 (□), 16×16 (△), 32×32 (◇), 64×64 (¤) and 100×100 (⊠) lattices.

in the half and full plane respectively, then we can write

$$\text{LT:} \quad \frac{1}{\pi}\int_{-\pi/2}^{\pi/2} \cos(\theta)\,\mathrm{d}\theta = 2/\pi \approx 0.637$$

$$\text{HT:} \quad \frac{1}{2\pi}\int_{-\pi}^{\pi} \cos(\theta)\,\mathrm{d}\theta = 0.$$

This behaviour is consistent with the behaviour of the largest lattice for the step model (shown in figure 3(*b*)).

Since the planar model has no conventional long range order we have that

$$\lim_{n\to\infty} C(n/2) = \begin{cases} 1 & \text{for } T = 0 \\ 0 & \text{for } T > 0. \end{cases} \tag{1}$$

However, since we are only dealing with finite lattices we are concerned with how this limiting behaviour is approached. Using the parametrisation of Tobochnik and Chester (1979) we can write

$$C(n/2) \sim (n/2)^{-T/2\pi} \begin{cases} \exp(-n/2\xi) & \text{for } T > T_c \\ 1 & \text{for } T < T_c. \end{cases}$$

For large fixed n we expect some smeared 'step function' behaviour for the { } factor modified by $(n/2)^{-T/2\pi}$ which is small but slowly varying in T near $T = T_c$. As n increases, the underlying 'step function' will get sharper, but the modulating factor $(n/2)^{-T/2\pi}$ will get smaller, resulting in the above limiting behaviour (equation (1)). So, while long range correlations are indeed destroyed by spin waves, it should still be possible to see evidence of a massive/massless phase transition when we consider $C(n/2)$ on a finite system.

In the case of the planar model then, we would argue that the increasingly sharp and converging contours shown in figure 3(*a*) are consistent with a phase transition. The contours shown in figure 3(*b*) for the step model are more difficult to interpret. The behaviour, however, does appear to be different from that shown in figure 3(*a*), and there is less evidence of either convergence or sharpening 'step function' behaviour.

We studied the susceptibility χ given by

$$\chi = \beta\tilde{\chi} = (\beta/N)(\langle M^2\rangle - \langle M\rangle^2).$$

We know that for an infinite system the spontaneous magnetisation $\langle M\rangle = \langle \cos\theta\rangle$ of the planar model is zero. For a finite system we find $\langle M\rangle$ small enough that it can be ignored. This was also found to be the case for the step model. We therefore only need calculate $\tilde{\chi} \approx (1/N)\langle M^2\rangle$. This function was also studied by both Miyashita *et al* (1978) and Tobochnik and Chester (1979).

Miyashita *et al* (1978) arrived at a critical temperature $kT_c/J \approx 1.15$ by examining the lattice size dependence of the susceptibility, T_c being marked by the transition from non-extensive to extensive behaviour. In contrast Tobochnik and Chester (1979) found a much lower critical temperature $kT_c/J = 0.89$ by fitting the correlation function and susceptibility data (at five temperature values between 1.0 and 1.2) to the Kosterlitz-Thouless form.

We would be far more cautious about using the susceptibility data to determine critical behaviour. In spite of using runs of over 60 000 sweeps near the critical temperature, we found the data to be poorly behaved. We can see this poor behaviour in tables 1 and 2 of Tobochnik and Chester (1979) where, for example, at $T = 1.15$ they found that when the system was being cooled $\langle M^2\rangle = 123$, but in the heating phase, at the same temperature, $\langle M^2\rangle = 61$.

A second method of calculating the susceptibility is simply to sum the correlation function over the box size, i.e.

$$\chi = \sum_{i=1}^{n} C(i).$$

While the data generated using this method were found to be better behaved, we still did not feel it was possible to use these data to support an argument for or against a phase transition in the case of the step model, or to determine the critical temperature in the case of the planar model.

A time series analysis (see Berretti and Sokal 1985) was carried out on the generated data points for the step and planar models. The aim of this analysis was to measure the degree of independence of the data, and thereby estimate the equilibration time of the system and the standard errors of each of the thermodynamic variables. The basis of this analysis is the calculation of the autocorrelation function

$$F(t)=\frac{1}{l-t}\sum_{i=1}^{l-t}(x_i-\bar{x})(x_{i+t}-\bar{x}_{i+t})/s_i s_{i+t}$$

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

$$\bar{x}_i=\sum_{i=1}^{l-t}x_i/(l-t)$$

$$\bar{x}_{i+t}=\sum_{j=t+1}^{l}x_j/(l-t)$$

and

$$s_k=(\overline{x_k^2}-\bar{x}_k^2).$$

The autocorrelation time t_a is the shortest time $t=t_a$ such that $F(t_a)<0.1$. Obviously $F(0)=1$. If all the data points are (pseudo)random, then $F(t)$ is found to have approximately 10% noise (and hence the above limit) and $t_a\approx 1$. The larger the value of t_a, the greater the correlation between the data. In practice, values of $F(t)$ for $t>3l/4$ become increasingly meaningless as $t\to l-1$. This, however, was not a problem in estimating t_a since in most cases we found that $t_a<100l$.

At each temperature up to 10 blocks of 2000 sweeps were carried out. For each block the value of t_a was calculated. Not surprisingly the largest estimates of t_a were obtained in the temperature range 0.8 to 1.5, the same interval over which the specific heat (figure 2) has maximum gradient. For higher temperatures, the energy was essentially uncorrelated with $t_a\approx 2$, and for lower temperatures $t_a\approx 10$. At each temperature, having determined a value for t_a, the average energy was calculated by choosing every t_ath data point. In table 1 we list step model and planar model energy data with standard errors calculated by using

$$s=\left(\sum_{i=1}^{m}(E_i-\bar{E})^2/m(m-1)\right)^{1/2}$$

where m is the number of sweeps, E_i is the energy of a given configuration and $\bar{E}$ is the average energy. We also calculated the autocorrelation function for the magnetisation. The behaviour, however, was erratic and inconclusive.

Tobochnik and Chester (1979) also calculated standard deviations of their energy data, by simply averaging blocks of 200 sweeps, and calculating the standard deviation of these averages. Unlike the above autocorrelation analysis, however, their method takes no account of the increasing equilibration time of the system as the 'critical temperature' is approached (also called critical slowing down).

Table 1. Comparison of the energy per spin and its standard error for the step and planar models on the 8×8 and 32×32 lattices.

	Step model				Planar model			
T	8×8 energy	s	32×32 energy	s	8×8 energy	s	32×32 energy	s
0.25	−2.000	0.000	−2.000	0.000	−1.873	0.000	−1.870	0.006
0.50	−1.987	0.000	−1.986	0.001	−1.735	0.000	−1.730	0.012
0.60	−1.972	0.001	−1.972	0.005	−1.674	0.001	−1.670	0.066
0.70	−1.953	0.001	−1.951	0.008	−1.604	0.000	−1.600	0.024
0.80	−1.925	0.001	−1.922	0.010	−1.540	0.000	−1.535	0.047
0.90	−1.886	0.002	−1.884	0.013	−1.457	0.001	−1.441	0.060
1.00	−1.835	0.002	−1.840	0.016	−1.359	0.002	−1.324	0.102
1.10	−1.801	0.007	−1.782	0.058	−1.233	0.002	−1.180	0.019
1.20	−1.719	0.009	−1.693	0.067	−1.114	0.002	−1.041	0.018
1.30	−1.653	0.011	−1.586	0.082	−0.993	0.005	−0.941	0.017
1.40	−1.535	0.004	−1.499	0.030	−0.905	0.016	−0.851	0.053
1.50	−1.457	0.005	−1.403	0.027	−0.807	0.015	−0.774	0.055
1.60	−1.367	0.005	−1.328	0.031	−0.726	0.014	−0.715	0.026
1.70	−1.274	0.002	−1.246	0.012	−0.676	0.015	−0.663	0.022
1.80	−1.194	0.002	−1.177	0.011	−0.633	0.014	−0.620	0.025
1.90	−1.144	0.002	−1.114	0.011	−0.591	0.012	−0.579	0.024
2.00	−1.064	0.002	−1.055	0.012	−0.540	0.013	−0.550	0.004
2.25	−0.929	0.002	−0.936	0.011	−0.458	0.012	−0.477	0.004
2.50	−0.824	0.001	−0.836	0.005	−0.428	0.004	−0.426	0.004
2.75	−0.755	0.001	−0.754	0.005	−0.387	0.004	−0.384	0.004
3.00	−0.693	0.001	−0.687	0.005	−0.351	0.004	−0.347	0.004

For the planar model we find a specific heat peak at $T\approx1.1$ which is in good agreement with Miyashita *et al* (1978). We are also in agreement with regard to the qualitative behaviour of the susceptibility. We do not, however, consider these data reliable enough to locate the critical temperature in the infinite lattice limit. For the step model the behaviour of the susceptibility is inconclusive.

Neither the step model nor the planar model show any evidence of hysteresis. The behaviour of the specific heat also appears to be lattice size independent for both models. While it is possible to interpret the behaviour of $C(n/2)$ for the planar model as supporting the existence of a critical point (at some $T<1.0$), this same interpretation does not appear possible for the step model. Since we 'know' that the step model does not undergo a topologically induced phase transition as is found in the planar model, we conclude that it is unlikely that the step model undergoes a phase transition. We should qualify this, however, by saying that numerical difficulties in the Monte Carlo procedure tend to obscure the differences that exist in the critical behaviour of the step and planar models.

The conclusion that there is no phase transition in the step model is consistent with the work of Barber (1983) who carried out a Migdal renormalisation group transformation on a number of O(2) spin systems including the step and planar models. For the planar model the Migdal transformation clearly identifies a high and low temperature phase, in contrast to the step model, where only one (disordered) phase can be identified.

Barber (1983) also studied the modified step model defined using the interaction function

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

$$C(\theta+2\pi)=C(\theta).$$

He found the behaviour of the Migdal transformation changed dramatically between the ordinary step model and the modified step model with $\delta<\frac{1}{2}$. He suggests that this model may indeed undergo a phase transition of some type, or alternatively, that this behaviour is the result of some artefact of the Migdal scheme.

We are currently studying the modified step model using Monte Carlo methods. This model is particularly interesting in the light of very recent Monte Carlo work by Domany *et al* (1984) and Van Himbergen (1984) on a modified planar model, defined using the interaction function

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

For $p\geqslant 3$ this model is found to undergo a far stronger (first-order) phase transition than the planar model. Note that increasing p in the modified planar model has the same effect as decreasing δ in the modified step model, i.e. it decreases the width of the well in the interaction function. This work will shortly be reported.

We would like to thank Professor A J Guttmann and Professor A D Sokal for stimulating discussions and constructive criticisms. In particular we would like to thank Professor Sokal for his very helpful suggestions regarding the statistical analysis and worth of Monte Carlo data.

References

Barber M N 1983 *J. Phys. A: Math. Gen.* **16** 4053
Berretti A and Sokal A D 1985 *J. Stat. Phys.* submitted
Domany E, Schick M and Swendsen R H 1984 *Phys. Rev. Lett.* **52** 1535
Fucito F 1983 *Phys. Lett.* **94A** 99
Fucito F and Solomon S 1983 *Phys. Lett.* **134B** 235
Guttmann A J 1978 *J. Phys. A: Math. Gen.* **11** 545
Kosterlitz J M and Thouless D J 1973 *J. Phys. C: Solid State Phys.* **6** 1181
Mermin N D and Wagner H 1966 *Phys. Rev. Lett.* **17** 1133
Metropolis N, Rosenbluth A W, Rosenbluth M N and Zeller A H 1953 *J. Chem. Phys.* **21** 1089
Miyashita S, Nishimori H, Kuroda A and Suzuki M 1978 *Prog. Theor. Phys.* **60** 1669
Nymeyer A and Guttmann A J 1985 *J. Phys. A: Math. Gen.* **18** 495
Tobochnik J and Chester G V 1979 *Phys. Rev.* B **20** 3761
Valleau J P and Whittington S G 1977 in *Statistical Mechanics* ed Bruce J Berne (New York: Plenum)
Van Himbergen J E 1984 *Phys. Rev. Lett.* **53** 5