Monte Carlo simulation of a planar Ising model roughening transition

1981 J. Phys. A: Math. Gen. 14 2059

(http://iopscience.iop.org/0305-4470/14/8/028)

J. Phys. A: Math. Gen. **14** (1981) 2059–2071. Printed in Great Britain

Monte Carlo simulation of a planar Ising model roughening transition

D B Abraham† and E R Smith

Mathematics Department, University of Melbourne, Parkville, Victoria, Australia 3052

Received 7 January 1981

Abstract. We report Monte Carlo simulations of a 65×65 planar square Ising model with boundary conditions chosen to allow examination of the roughening transition recently described by Abraham. Magnetisation profiles in excellent agreement with the known exact result were obtained. Equilibrium spin pair correlation functions are described: those across the interface which is established show anomalously long-ranged effects. The spin autocorrelation functions show anomalously slow decay.

1. Introduction

The interface between two coexisting pure phases in fluids, binary mixtures and uniaxial ferromagnets has been the subject of much recent scrutiny. There has been a remarkably successful phenomenological theory due to van der Waals (1894), culminating in the work of Widom and his collaborators (Fisk and Widom 1969). This is based on an assumed free energy density functional of the density profile established in an inhomogeneous system. The total free energy is then minimised by calculus of variations to obtain the equilibrium profile, which is found to vary on the scale of the correlation length ξ for a pure phase. The notion that the characteristic length is in fact ξ led Widom to the first scaling law for critical exponents (Widom 1965).

Statistical mechanical theories at atomic dimensions make suggestions which modify the free energy density theory at a fundamental level. But such theories are far from complete. For instance, there is not even a *general* proof of existence of phase transitions (Ruelle 1971) for continuous systems. On the other hand, lattice gases have two advantages: firstly, *mutatis mutandis* the same theory treats gases, uniaxial ferromagnets and binary mixtures and alloys. Secondly, there are many mathematically exact results. Provided the correlation length ξ is large on the scale of the interaction range, assumed finite, we may expect the lattice gas theory to be essentially exact for continuous systems. We now continue with a résumé of relevant exact results for lattice systems.

Imagine a cubical volume V to be divided up into small cells of size a. At the centre of each cell, labelled i, there is a spin $\sigma(i) = \pm 1$. The cubical lattice formed by the centre points i is denoted Λ. A spin configuration, denoted $\{\sigma\}$, on Λ has an energy

$$E_\Lambda(\{\sigma\}) = -\tfrac{1}{2} \sum_{\substack{i,j \in \Lambda \\ i \neq j}} J(i,j)\sigma(i)\sigma(j) - \sum_{i \in \Lambda} H(i)\sigma(i) \tag{1}$$

† On leave from Oxford University.

0305-4470/81/082059+13$01.50

where $J(i, j)$ ($\geqslant 0$) is a ferromagnetic coupling. This coupling is zero unless i and j are nearest neighbours, when $J(i, j) = J$. Equation (1) also contains a magnetic field $H(i)$. The probability of such a configuration is

$$p_\Lambda(\{\sigma\}) = Z_\Lambda^{-1} \exp[-\beta E_\Lambda(\{\sigma\})] \tag{2}$$

where Z_Λ is the canonical partition function which normalises (2) and $\beta = 1/kT$ is the usual notation.

The first key result is that if we take a cubical region Λ centred on the origin and surrounded by spins all constrained to be $+1$, then provided the dimension $d \geqslant 2$, there exists $T_p(d)$ such that for $0 < T < T_p(d)$ and for $H(i) = 0$

$$\lim_{\Lambda \to \infty} \langle \sigma(0) \rangle_{\Lambda,+} = m^* \tag{3}$$

with $m^* > 0$. The average $\langle\ \rangle_{\Lambda,+}$ is taken with respect to (2) with the constraint $\sigma(i) = +1$ outside Λ. If the constraint is reversed then m^* carries a factor -1 in (3). This result, due to Peierls (1936) and improved by Dobrushin (1968) and Griffiths (1964), shows that these models are *unstable with respect to boundary conditions* at low enough temperatures. This view of a phase transition complements the usual one in terms of the free energy. The mechanism of proof is illuminating. Unit line segments for $d = 2$ (unit squares for $d = 3$) are drawn between all neighbouring pairs of spins having opposite sign. We thus obtain contours which are edge self-avoiding and cannot terminate inside Λ; at intersections only 0, 2 or 4 line segments may meet. When the boundary conditions + or − are imposed, no contours intersect the boundary of Λ. For $d = 3$ the contours are closed polygonal sheets. Let the area (volume for $d = 3$) of Λ be denoted $|\Lambda|$. The contours are treated perturbatively to show that the total area contained within contours grows as $|\Lambda|$, but the proportionality can be made as small as desired by taking T small enough. Also, the total length of any contour is smaller than $\ln|\Lambda|$ with probability one. Thus we capture the idea of *small* contours of reversed magnetisation disordering a pure phase.

This result may be generalised as follows: consider collections of points A which have finite diameter on the lattice and let

$$\sigma(A) = \prod_{i \in A} \sigma(i). \tag{4}$$

Then no matter what the boundary conditions on Λ are, if we consider those $\langle \sigma(A) \rangle$ which are translationally invariant on Λ as $\Lambda \to \infty$, there exists $\lambda \in [0, 1]$ such that

$$\lim_{\Lambda \to \infty} \langle \sigma(A) \rangle_\Lambda = \lambda \langle \sigma(A) \rangle_+ + (1 - \lambda) \langle \sigma(A) \rangle_- \tag{5}$$

where $\langle \sigma(A) \rangle_\pm$ is the infinite volume limit with either + or − boundary conditions. The same λ obtains for all A. This result interprets the disproportionation along the tie lines but it tells us little of the typical geometric relations between phases.

It is natural to investigate this problem by taking boundary conditions on a box $\Lambda = \{(x)_{d-1}, z | -N + 1 \leqslant z \leqslant N, -M \leqslant x_j \leqslant M, j = 1, \ldots, d-1\}$ such that $\sigma(i) = +1$ (-1) on the boundary if $z > 0$ $(\leqslant 0)$. Then, as $N, M \to \infty$, the magnetisation will be $+m^*$ at the centre of the upper half box, and $-m^*$ for the lower one. These two regions will be separated by a long contour or sheet which intersects the surface of Λ at $z = \frac{1}{2}$. When $d = 2$, Gallavotti (1972) proved that for $T < T_G \ll T_c(2)$ (where $T_c(d)$ is the d-dimensional critical temperature), with probability one as $N \to \infty$, the long contour is at least as far as M^δ from any finite region, with $\delta < \frac{1}{2}$. Thus we may reasonably infer that

$\langle\sigma(0, p)\rangle_\infty = 0$ for all finite p. This result has recently been supplemented for $d = 2$ by Higuchi (1979) and Aizenman (1979, 1980) who proved that all $\langle\sigma(A)\rangle_\infty$ are translationally invariant for all $T < T_c(2)$.

On the other hand, for $d = 3$, Dobrushin (1972) showed that the magnetisation $\langle\sigma(0, p)\rangle_\infty$ varies with p, the region of validity for this being extended to $0 \leqslant T < T_c(2)$ by van Beijeren (1975). This bound has a simple motivation in the Burton–Cabrera–Frank theory (1951): the interface behaves like a $d = 2$ Ising model with no field, since that arising in mean field theory from above and below cancels out by symmetry. Indeed, Weeks *et al* (1973) suggested that at a temperature T_R not discernibly different from $T_c(2)$, there is a phase transition to an intermediate phase on $(T_R, T_c(3))$ which has a strongly fluctuating interface and $\langle\sigma(0, p)\rangle_\infty = 0$ for all $|p| < \infty$. The fluid region of the phase diagram is therefore likely to lie within the fluctuating region, certainly so near criticality. Thus for both $d = 2$ and $d = 3$ we have results totally at variance with theories based on free energy functionals, and, moreover, with everyday experience. Furthermore, the existence of a phase transition entails, in accordance with accepted phenomenology, an *additional* correlation length which diverges at T_R; this is contrary to accepted dogma, since there should be concomitant singularities in other quantities, which are not observed. In the remainder of this section we summarise some relevant exact results recently obtained for $d = 2$ which form a basis for the Monte Carlo simulations which we report in this paper.

For $d = 2$ we have the exact result (Abraham and Reed 1974, 1976)

$$\lim_{M\to\infty}\lim_{N\to\infty}\langle\sigma(0, \alpha M^\delta)\rangle_{N,M} = \begin{cases} 0, & \delta < \frac{1}{2}, \\ m^* \operatorname{sgn}\alpha\, \Phi(b|\alpha|), & \delta = \frac{1}{2}, \\ m^* \operatorname{sgn}\alpha, & \delta > \frac{1}{2}, \end{cases} \tag{6}$$

where

$$\Phi(x) = \frac{2}{\sqrt{\pi}}\int_0^x \exp(-u^2)\,du \tag{7}$$

and

$$b = (\sinh\gamma(0))^{1/2} \tag{8}$$

with $\gamma(0)$ the real positive root of

$$\cosh\gamma(\omega) = (\cosh 2K)^2/\sinh 2K - \cos\omega, \tag{9}$$

a celebrated formula due to Onsager (1944). This result indicates where the interface is likely to be found and ties in nicely with Gallavotti's theorem. It is interesting to recall that $\gamma(0)$ is the surface tension in units of kT (Onsager 1944). Let us define for $n \geqslant 0$

$$S(n) = \sum_{p=0}^{\infty} p^n m^*[1 - \Phi(bp/M^{1/2})]. \tag{10}$$

Then the RMS width of the interface, denoted l_2, is

$$l_2 = a_0(S(2)/S(0))^{1/2} \tag{11}$$

where a_0 is the side length of a lattice cell, typically the range of the potential. Combining (6), (7) and (8) it is evident that

$$l_2 \sim a_0(M/\gamma(0))^{1/2}. \tag{12}$$

This formula also occurs in the Buff *et al* (1965) theory developed for $d=2$. Its numerical consequences are striking. Recall that $\xi \sim 1/\gamma(0)$ in lattice units. If $M/\gamma(0) \sim 10^8$, which is typical, then $l_2 \sim 10^{-4}$ cm. Such an effect would not be observable without optical leverage. Thus doubts as to the completeness of the statistical mechanical theory based on everyday observation cannot be sustained.

A modified form of the above model, which we shall now describe, has a roughening transition at a temperature which can be made as close as one wishes to $T_c(2)$. Thus it may be experimentally observable.

Consider the strips $\Lambda = \{(x, z), 0 \leqslant x \leqslant N+1, -\infty < z < \infty\}$ with boundary conditions $\sigma(N+1, z) = +1$, $\sigma(0, z) = -1$ if $-S \leqslant z \leqslant S$, $+1$ if $|z| > S$. This produces a single long contour. Let the horizontal bond strength between spins in columns 0 and 1, normally J, be replaced by aJ with $0 < a < 1$. The long contour thus experiences an attraction to the line $x = \frac{1}{2}$ which conflicts with the maximisation of entropy in establishing equilibrium. The phase diagram is shown in figure 1 (Abraham 1980). In the fluctuating region the profile obeys

$$\lim_{s\to\infty} \lim_{N\to\infty} \langle \sigma(\alpha s^{\delta}, 0)\rangle = \begin{cases} -m^*, & \delta < \frac{1}{2}, \\ m^* F[(2b\alpha)^{1/2}], & \delta = \frac{1}{2}, \\ m^*, & \delta > \frac{1}{2}, \end{cases} \tag{13}$$

where b is given by (8) and

$$F(x) = 1 - \frac{4}{\sqrt{\pi}}\left(x \exp(-x^2) - \int_x^{\infty} \exp(-t^2)\, dt \right). \tag{14}$$

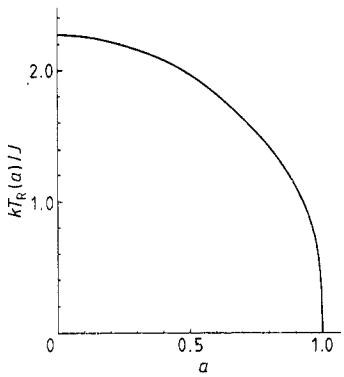

Figure 1. Phase diagram for roughening transition: plot of a_c against T or C_c against A.

This result, originally obtained when $a = 1$ (Abraham and Issigoni 1979), is *independent of a* in the fluctuating region. Also, on the scale of the spacing

$$\lim_{s\to\infty} \lim_{N\to\infty} \langle \sigma(p, 0)\rangle = -m_+(p) \tag{15}$$

where $m_+(p)$ is the profile which obtains when $\sigma(0, x) = \sigma(N+1, x) = +1$ for all x. The decay here is on a length scale of the bulk correlation length $\xi = 1/\gamma(0)$.

In the region of the phase diagram with the contour bound, we have

$$\lim_{s\to\infty} \lim_{N\to\infty} \langle \sigma(p, 0)\rangle = F(p, a, T) m_+(x) \tag{16}$$

where $F(0, a, T) = -1$, $F(\infty, a, T) = 1$ and the length scale in F is $1/\gamma(iv_0)$, where $\gamma(\omega)$ is given by (9) and

$$\cosh v_0 = \tfrac{1}{2}(B + 1/B) + 1 = \tfrac{1}{2}(w + 1/w) \tag{17}$$

with

$$B = e^{-2K} \cosh K \tag{18}$$

and

$$w = e^{2K}(\cosh 2K - \cosh 2aK)/\sinh 2K. \tag{19}$$

The aim of this paper is to simulate this system using the Monte Carlo method. The existence of an exact solution for some aspects of the problem has enabled us to handle with confidence a problem with up to three length scales. We obtain static pair correlation functions in both regions, giving evidence of anomolously long range in the actual region of transition, which is localised due to the finite value of s. Our simulation uses an associated Markov chain with Glauber dynamics (Glauber 1963); we can thus obtain equilibrium autocorrelation functions and evidence of long-time tails in the interface region. In the next section we shall describe our method and results. The paper will conclude with a discussion.

2. Simulation results

We report simulations of a 65×65 nearest-neighbour square lattice Ising model. The lattice is wrapped on a cylinder so that the spins $\sigma(i, j)$ are periodic in j with period 65. The boundary spins $\sigma(65, j)$ are also coupled to an extra row of fixed + spins with coupling constant J, the coupling constant in the bulk of the lattice. The spins at the other boundary are also coupled to an extra row of fixed spins, but with coupling constant aJ, $0 < a < 1$. Of these fixed spins, those coupled to $\sigma(1, j)$ for $a \leqslant j \leqslant 57$ are $-$ while the rest are +. The simulations were carried out with zero applied field, although an alternative interpretation using (1) is that the surface spins are acted on by fields. For convenience we introduce the notation

$$A = e^{-2J/kT}, \qquad C = e^{-2aJ/kT}. \tag{20}$$

The critical value of A is $\sqrt{2} - 1$. We used $A = 0.35$ throughout; this gives a bulk correlation length of about 3, facilitating separation of length scales within the limitations of our simulation. The critical value of C for the roughening transition for $A = 0.35$ is $C \simeq 0.54$. We considered two values of C with a rough surface (0.4, 0.45) and two values of C with a bound surface (0.65, 0.8).

The simulations were considered as made up of 'moves' and 'time steps'. In a 'move', a spin on the square lattice was chosen randomly and then overturned using the Glauber dynamics algorithm (Glauber 1963). That is, if the change in energy on overturning a spin was ΔE, the spin was overturned in the move with probability

$$p = [1 + \exp(\Delta E/kT)]^{-1}. \tag{21}$$

If the spin was not overturned, the move consisted of changing nothing. A 'time step' was composed of 65^2 consecutive moves. The system was equilibrated for at least 10^4 time steps for each value of C. A run of 100 time steps was then done to store a history of 100 consecutive configurations $\{\sigma\}$. Averages of properties of the system were then

taken over 2×10^4 subsequent time steps. The equilibration runs for $C=0.8$ and $C=0.4$ (10^4 and 4×10^4 time steps, respectively) were started from configurations constructed by choosing each spin in turn to be + with probability $(1+m^*)/2$ and otherwise −. The equilibration run for $C=0.65$ (10^4 time steps) was started from the final configuration of the averaging run at $C=0.8$. The equilibration run at $C=0.45$ (10^4 time steps) was started from the final configuration of the averaging run at $C=0.4$. The averaging runs of 2×10^4 time steps consisted of 8.45×10^7 moves.

To define the correlation functions which we measured, let $\sigma(i,j|K)$ be the state of $\sigma(i,j)$ at the Kth time step of the averaging run. Note that $K\in(-99, 2\times10^4)$, because the averaging run was preceded by 100 time steps.

Our results fall into three categories. Firstly, we have endeavoured to approximate the exact results from theory for the magnetisation profile. In figure 2 we plot

$$m(i)=\frac{1}{10^5}\sum_{K=1}^{2\times10^4}\sum_{j=31}^{35}\sigma(i,j|K). \tag{22}$$

The sum on K divided by 2×10^4 is supposed to approximate the canonical equilibrium average (2). Our resources did not permit us to obtain data for the limiting procedure in (13) and (14). Nevertheless, for $C=0.4$ and $C=0.45$ we see in figure 2 a remarkable agreement with the theoretical function and a significant independence of C there, even with such small values of s (number of reversed spins in edge; $s=49$ in these simulations). The lack of precise agreement with the exact result is presumably due to the finite size of s. The exact results do not give any estimate of finite size corrections as yet. The contrast with $C=0.65$ and $C=0.8$ in figure 2 is most striking. In that case, the interface is bound to the edge on a length scale which evidently increases as C decreases

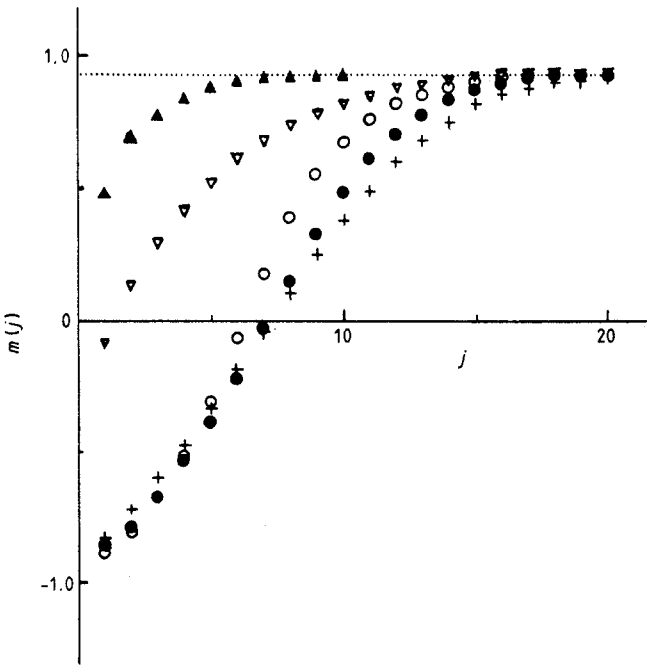

Figure 2. Plots of $m(i)$; ▲: $C=0.8$; ▽: $C=0.65$; ●: $C=0.45$; ○: $C=0.4$. +: result of (13).

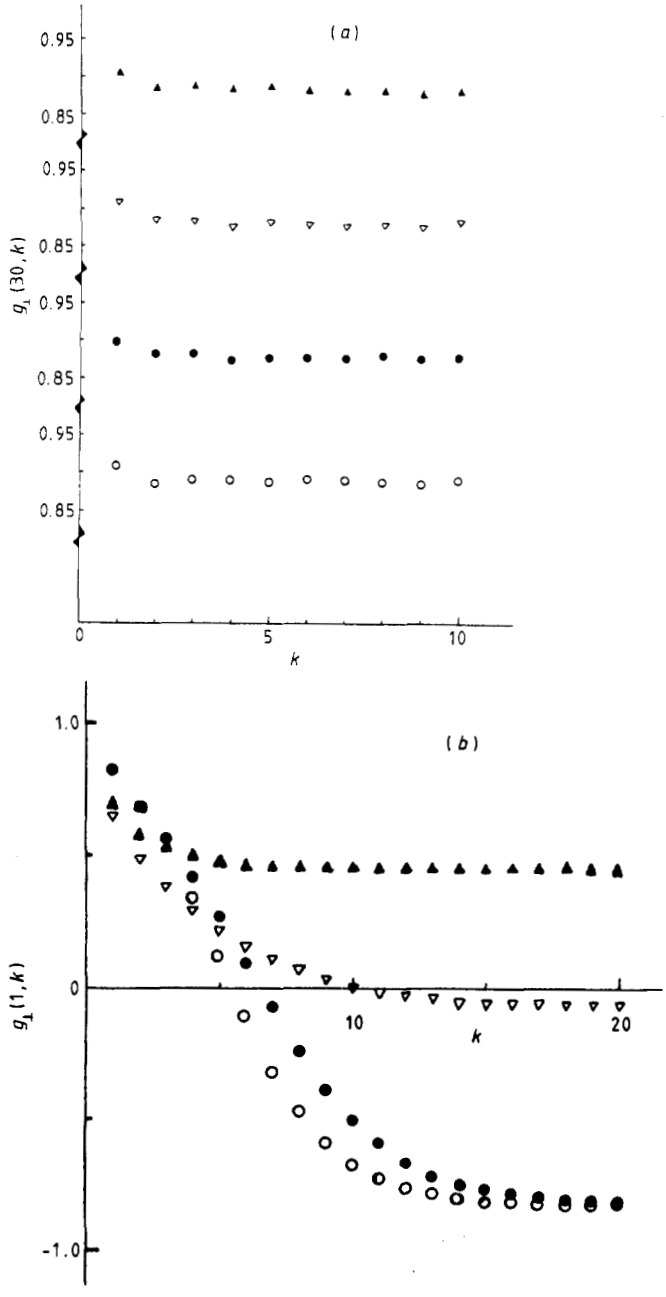

Figure 3. ▲: $C = 0.8$; ▽: $C = 0.65$; ●: $C = 0.45$; ○: $C = 0.4$. (*a*) Plots of $g_\perp(30, k)$. (*b*) Plots of $g_\perp(1, k)$.

towards its critical value, as expected. This picture is confirmed by typical configurations plotted in figure 6. The profiles for the larger values of C correspond to regions of $-$ spins bound to the fixed $-$ spins with a characteristic length of $1/\gamma(iv_0)$, with values ~ 4 for $C = 0.8$, ~ 10 for $C = 0.65$. For the smaller values of C the surface of the region of $-$ spins undergoes large fluctuations on a length scale $(s\xi)^{1/2} \sim 12$.

The use of an average over a strip of five spins perpendicular to the row of fixed overturned spins and in the middle of them requires some comment. During the rather long equilibration run at $C = 0.4$, magnetisation profiles

$$m(i; l) = \frac{1}{(2l+1)N} \sum_{K=1}^{N} \sum_{j=33-l}^{33+l} \sigma(i, j|K) \tag{23}$$

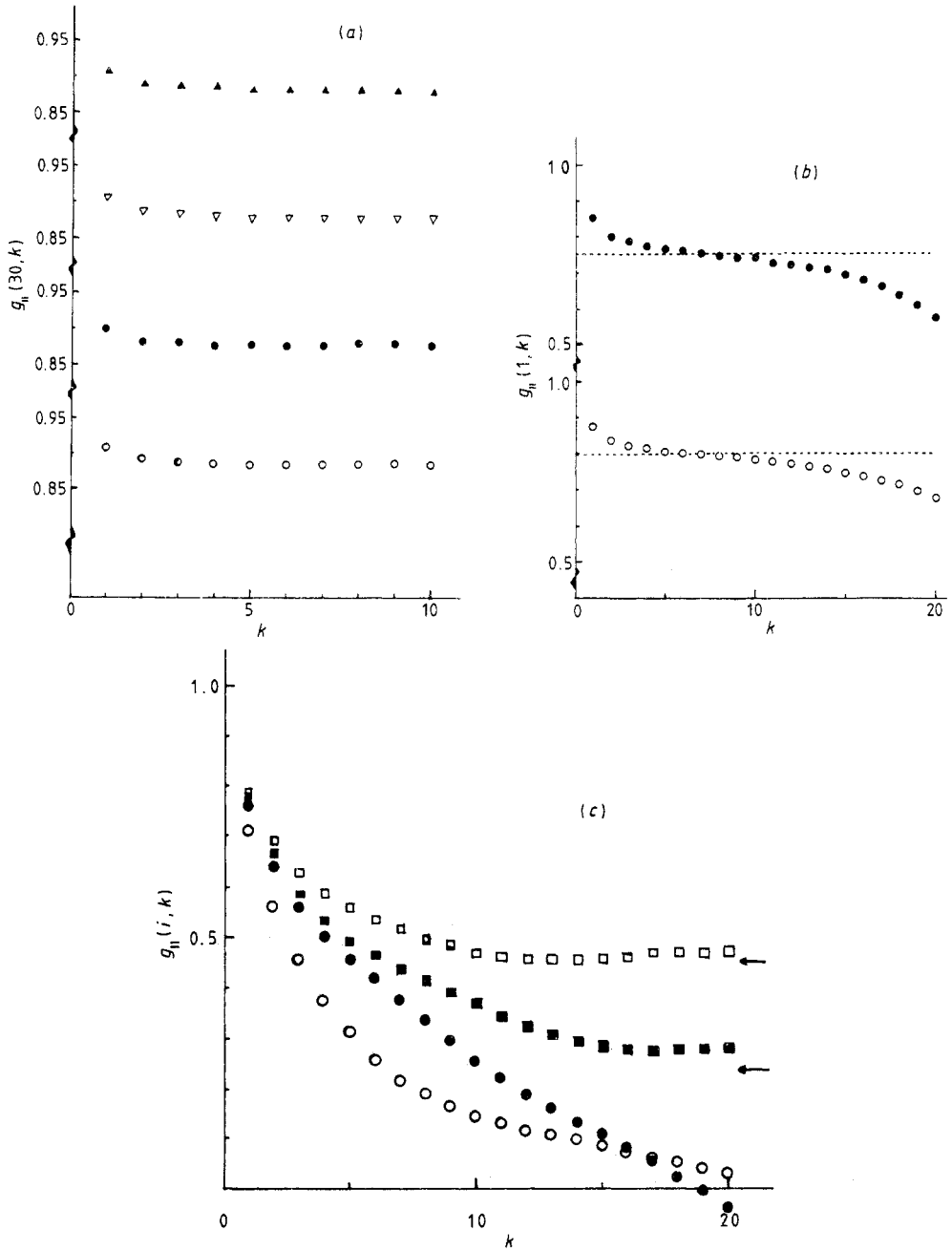

Figure 4.

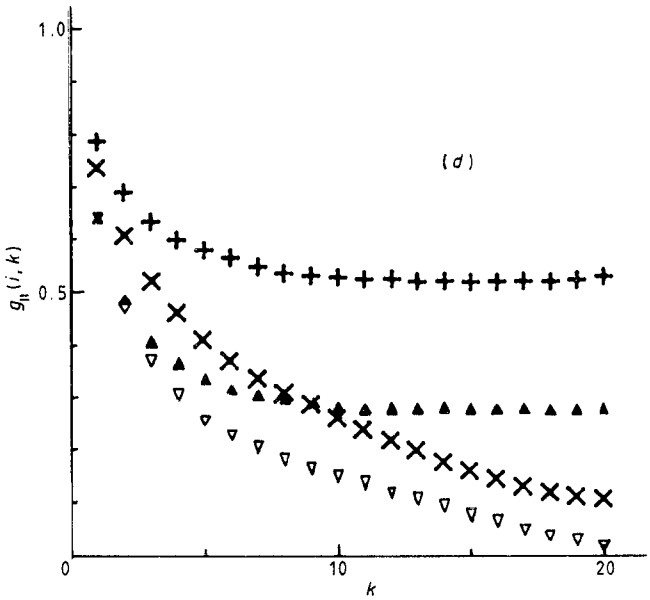

Figure 4. (*a*) Plots of $g_{\parallel}(30, k)$; ▲: $C = 0.8$; ▽: $C = 0.65$; ●: $C = 0.45$; ○: $C = 0.4$. (*b*) Plots of $g_{\parallel}(1, k)$; ●: $C = 0.45$; ○: $C = 0.4$. (*c*) Plots of $g_{\parallel}(i, k)$; ●: $C = 0.45$, $i = 6$; ○: $C = 0.4$, $i = 6$; ■: $C = 0.45$, $i = 9$; □: $C = 0.4$, $i = 9$. (*d*) Plots of $g_{\parallel}(i, k)$; ▲: $C = 0.8$, $i = 1$; ▽: $C = 0.65$, $i = 1$; +: $C = 0.8$, $i = 3$; ×: $C = 0.65$, $i = 3$.

were calculated for $l = 0$, 1, 2, 3 and 12 with $N = 10^4$. The results were rather 'noisy' for $l = 0$ and became smoother as l increased. However, while the profiles for $l = 2$, 3 and 12 were satisfactorily smooth, only the profile with $l = 2$ stayed close to the $l = 0$ profile. The larger values of l gave profiles which apparently reflected the fact that the profile at the edges of the row of overturned spins is not the same as that at the centre of this row. The choice of $l = 2$ seemed the best compromise between on the one hand requiring smooth data and, on the other, representing the profile at the centre of the row of overturned spins.

In the second category we have equilibrium pair correlation function results; none of these can yet be checked against theory. We have calculated

$$g_{\parallel}(i, k) = \frac{1}{2\times 10^5} \sum_{k=1}^{2\times 10^4} \sum_{j=31}^{35} \sigma(i, j|K)[\sigma(i, j+k|K) + \sigma(i, j-k|K)] \tag{24}$$

and

$$g_{\perp}(i, k) = \frac{1}{10^5} \sum_{k=1}^{2\times 10^4} \sum_{j=31}^{35} \sigma(i, j|K)\sigma(i+k, j|K). \tag{25}$$

In figure 3(*a*), we plot $g_{\perp}(30, k)$ with $k = 1, \ldots, 10$ for all the values of C. The results have no detectable C-dependence, as expected. They show the anticipated rather short correlation length $\xi/2 \sim 1.6$. The results in figure 3(*b*) for $g_{\perp}(1, k)$ are compatible with the profile expression (14). Dependence on C for $C = 0.4$ and 0.45 is only significant in the initial decay to $-m(1)m^*$ on a length scale of ξ, followed by the passage of k through

the interface region to achieve final decay to the value $m(1)m^*$. Notice that the correct final clustering values are obtained in all cases.

In figure 4(a) we give $g_{\|}(30, k)$ with $k = 1, \ldots, 10$ for all values of C. The plots are identical with those for $g_{\perp}(30, k)$, which is a necessary consequence of lattice isotropy. Figure 4(b) is a plot of $g_{\|}(1, k)$ for $C = 0.4$ and $C = 0.45$. The horizontal lines in these plots are at a height $m(1)^2$. These functions show a rapid decay within the average domain size to $m(1)^2$, followed by a much slower decay, presumably ultimately to $-m(1)^2$ for an infinite system. The necessary finite size of our simulation sample imposes a serious constraint here. The function $g_{\|}(i, k)$ is explored further in figure 4(c), which displays $g_{\|}(6, k)$ and $g_{\|}(9, k)$ for $C = 0.4$ and $C = 0.45$: $g_{\|}(9, k)$ decays rapidly to its clustering value on a length scale $\sim\xi$, but $g_{\|}(6, k)$, which refers to the typical interface region for the value of s used (see figure 2), decays much more slowly. Finally, in figure 4(d), $g_{\|}$ is examined for the bound interface at $C = 0.8$ and $C = 0.65$. For $C = 0.8$, both $g_{\|}(1, k)$ and $g_{\|}(3, k)$ decay to $m(1)^2$ or $m(3)^2$ on a short length scale up to $k = 20$. When $C = 0.65$, figure 2 shows that the interface has already broadened in anticipation of the roughening transition. There may well be two length scales operating here.

Our third category of result uses the Markov chain associated with the Ising problem in the simulation to generate time-dependent autocorrelation functions. We define

$$G_t(i|k) = \left\{ \frac{1}{10^5} \sum_{K=1}^{2\times 10^4} \sum_{j=31}^{35} \sigma(i, j|K)\sigma(i, j|K-k) \right\} - m(i)^2. \tag{26}$$

In figure 5(a) we plot $G_t(30|k)$ for all values of C. We see that there is an insignificant C-dependence. Figure 5(b) shows $G_t(1|k)$ for $C = 0.4$ and $C = 0.45$. Evidently within the domain there is another much longer time scale operating. This is also seen in figure 5(c) which shows $G_t(6|k)$ and $G_t(10|k)$ for $C = 0.4$ and $C = 0.45$.

Finally, we present in figures 6(a) and (b) two representative configurations. Figure 6(a) shows $\sigma(i, j|10^4)$ for $C = 0.65$ and figure 6(b) shows $\sigma(i, j|2\times 10^4)$ for $C = 0.45$. Figure 6(a) shows a few small clusters of $-$ spins bound to the row of fixed $-$ spins. Figure 6(b) shows a well developed region of $-$ spins attached to the row of fixed $-$ spins. The contour dividing this region from the bulk of the lattice is seen to have large-scale spatial fluctuations.

The use of an equilibration run of 10^4 time steps also deserves comment. It was found, for the initial states used with $C = 0.4$ and $C = 0.45$, that this length of equilibration run gave a magnetisation profile in excellent agreement with (14), so that information about the initial configuration had apparently been lost. The profiles measured in the subsequent 2×10^4 time step averaging runs did not differ significantly from those resulting from the equilibration runs.

3. Discussion

In summary, we have shown that our simulation reproduces with considerable accuracy known exact results for the roughening transition in the planar Ising model. We have not given any statistical analysis of our results since the usual naive treatment was at first quite misleading: stable results were obtained for runs of 10^3 time steps which nevertheless did not agree with (14). One of the difficulties here is the persistence of correlations with time in the interface region. Thus we regard the availability of exact results here as highly important.

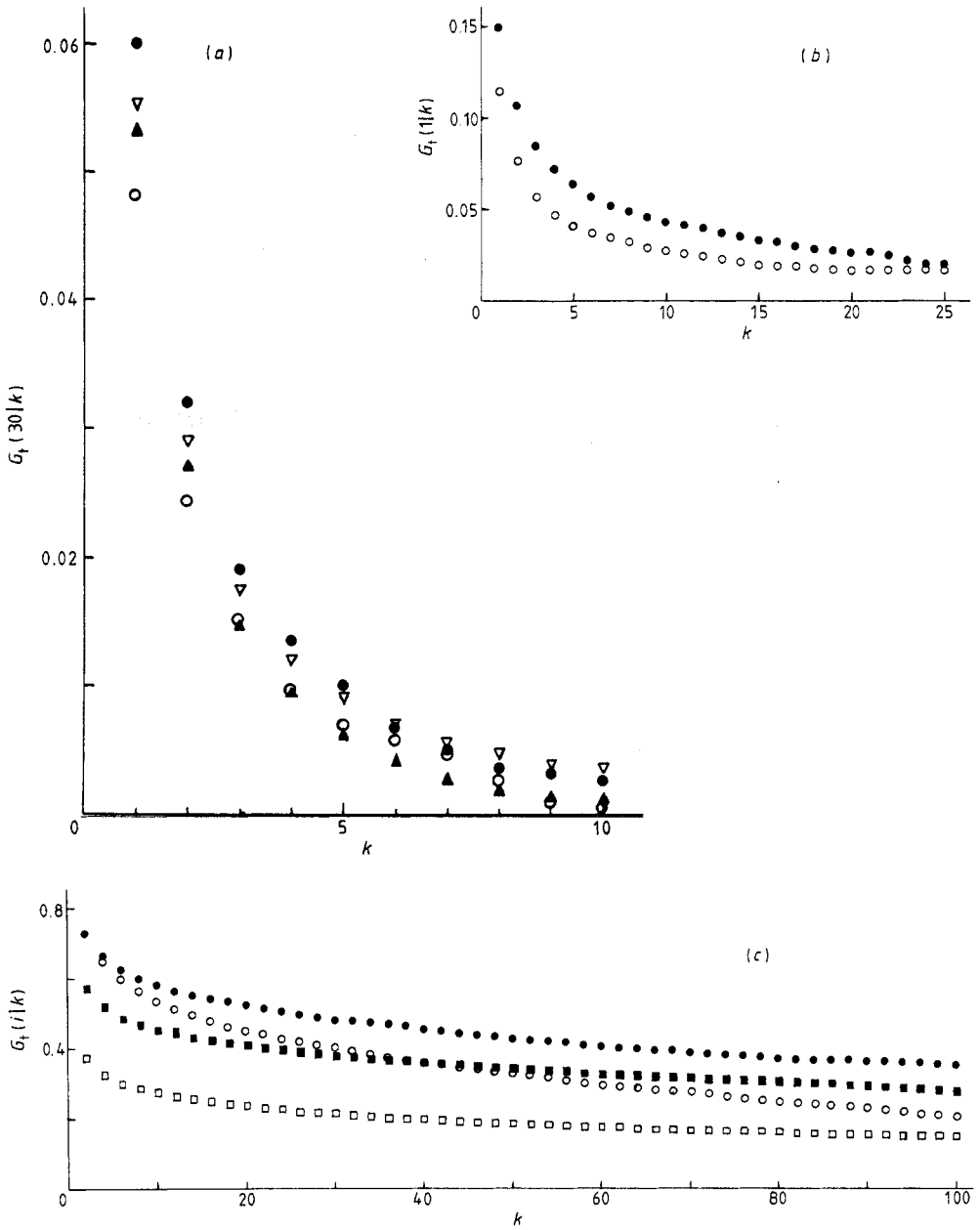

Figure 5. (*a*) Plots of $G_t(30|k)$; ▲: $C = 0.8$; ▽: $C = 0.65$; ●: $C = 0.45$; ○: $C = 0.4$. (*b*) Plots of $G_t(1|k)$; ● $C = 0.45$; ○: $C = 0.4$. (*c*) Plots of $G_t(i|k)$; ●: $C = 0.45$, $i = 6$; ■: $C = 0.45$, $i = 10$; ○: $C = 0.4$, $i = 6$; □: $C = 0.4$, $i = 10$.

Clearly much further work remains to be done on time-dependent phenomena. For instance, what effect does diffusive dynamics have? Are these characterisable metastable states? The motion of the interface may well have a diffusive character with such variables as $s/\sqrt{t}$ playing a role.

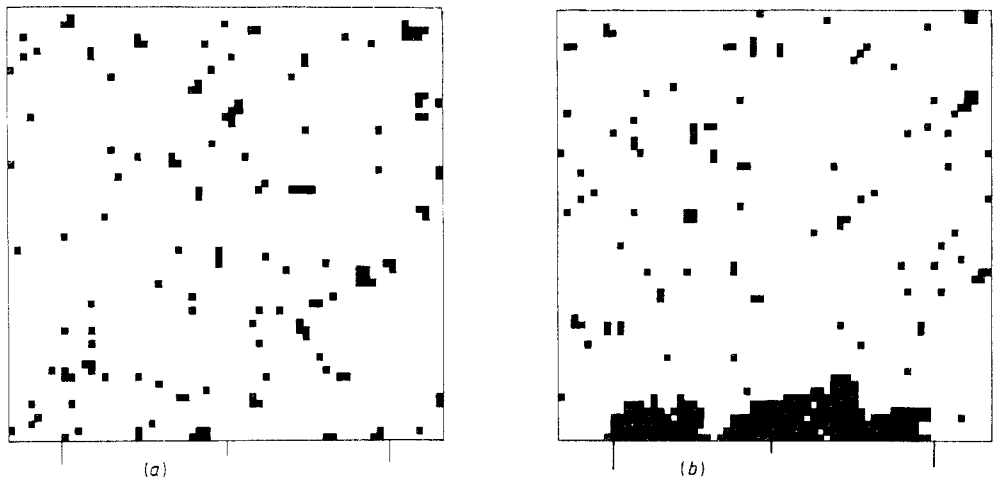

Figure 6. (*a*) Configuration $\sigma(i, j|10^4)$ for $C = 0.65$. Overturned (−) spins are represented by black squares. Bars on edge represent ends and middle of edge row of fixed overturned spins. (*b*) Configuration $\sigma(i, j|2 \times 10^4)$ for $C = 0.45$: markings as for (*a*).

The static pair correlation functions show evidence of the anomalous long-range decays suggested by Wertheim (1976) and Weeks (1977). Such phenomena occur only *in the interface*; we use the finite value of s to localise the domain wall effectively. It may ultimately prove possible to calculate $g_{\parallel}$ and $g_{\perp}$ exactly with leading finite-s corrections.

Acknowledgment

D B Abraham thanks the staff of the Mathematics Department of Melbourne University most cordially for their hospitality during his visit.

References

Abraham D B 1980 *Phys. Rev. Lett.* **44** 1165
Abraham D B and Issigoni M E 1979 *J. Phys. A: Math. Gen.* **13** L89
Abraham D B and Reed P 1974 *Phys. Rev. Lett.* **33** 377
—— 1976 *Commun. Math. Phys.* **49** 35
Aizenman M 1979 *Phys. Rev. Lett.* **43** 407
—— 1980 *Commun. Math. Phys.* **73** 83
van Beijeren H 1975 *Commun. Math. Phys.* **40** 1
Buff F P, Lovett R A and Stillinger F H 1965 *Phys. Rev. Lett.* **15** 621
Burton W K, Cabrera N and Frank F C 1951 *Phil. Trans. R. Soc.* A **243** 299
Dobrushin R L 1968 *Funct. Anal. Appl.* **2** 292, 302
—— 1972 *Theory Prob. Appl.* **17** 582
Fisk S and Widom B 1969 *J. Chem. Phys.* **50** 3219
Gallavotti G 1972 *Commun. Math. Phys.* **27** 103
Glauber R J 1963 *J. Math. Phys.* **4** 294
Griffiths R B 1964 *Phys. Rev.* **136A** 437
Higuchi Y 1979 *Colloquium on Random Fields*
Onsager L 1944 *Phys. Rev.* **65** 117

Peierls R E 1936 *Proc. Camb. Phil. Soc.* **32** 477
Ruelle D 1971 *Phys. Rev. Lett.* **27** 1040
van der Waals J D 1894 *Z. Phys. Chem.* **13** 657
Weeks J D 1977 *J. Chem. Phys.* **67** 3106
Weeks J D, Gilmer G H and Leamy H J 1973 *Phys. Rev. Lett.* **31** 549
Wertheim M S 1976 *J. Chem. Phys.* **65** 2377
Widom B 1965 *J. Chem. Phys.* **43** 3892