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Universal finite-size scaling amplitudes on a torus for the triangular Ising lattice gas

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Abstract. Recently we suggested studying the scaling properties of complex two-dimensional phase transitions by calculating the universal amplitudes of interfacial free energies on a torus geometry employing Monte Carlo simulations. Here we test this method at the $\sqrt{3} \times \sqrt{3}$ phase transition in the Ising lattice gas on a triangular lattice belonging to the chiral three-state Potts universality class. The interfacial free energies for this lattice gas model can be written in terms of free energy differences between systems with different sizes. The algorithm to calculate these free energy differences is presented. Using lattice sizes up to 18×18 and modest computing effort, we find that the universal amplitude $A = 1.22 \pm 0.02$, in accordance with the exact analytical value for the non-chiral three-state Potts model, $A = 1.203291\cdots$, which we determined earlier.

Finite-size scaling (FSS) is an important tool in numerical investigations of critical phenomena. In particular, the finite-size scaling behaviour of interfacial free energies and correlation lengths is very useful. Recently, the exact relationship between the values of critical exponents and universal finite-size scaling amplitudes of correlation lengths and interfacial free energies has been established for two-dimensional phase transitions. This was first done for semi-infinite strip geometries (see e.g. Luck 1982 and Cardy 1984). More recently we generalised this to torus geometries for transitions in the Potts model universality class (Park and den Nijs 1988).

In the case of semi-infinite lattices (using the transfer matrix method) these relationships lead to very accurate numerical results for the critical exponents (see e.g. Blöte and Nightingale 1985, Blöte and den Nijs 1988). However, the transfer matrix method is limited to small strip widths. It is possible to obtain the exact free energy of semi-infinite strips only for widths up to about $N = 18$ (for Ising type models with two states per site). There are many interesting problems where the asymptotic scaling behaviour will not set in until larger lattice sizes; for example in systems with incommensurate domain wall networks (Park *et al* 1986). For large lattice sizes approximate methods such as Monte Carlo simulations are the only remaining option. For this purpose, and guided by the fast convergence of the FSS method on semi-infinite strips, we set out to develop and test a Monte Carlo version of the above FSS type analysis of universal amplitudes for interfacial free energies (Park and den Nijs 1989).

In MC simulations the lattice is finite in both directions: a torus instead of a semi-infinite strip. The relationship between the critical exponents and the universal amplitudes of the interfacial free energies is more complex than in the cylinder geometry, but this exact relationship has been determined analytically in the case of the Potts

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model universality class (Park and den Nijs 1988). In principle this can be extended to most other 2D universality classes (Saleur 1987, Park and Widom 1989, 1990).

In an earlier paper (Park and den Nijs 1989) we introduced this MC method and presented our initial test results. We applied the method to the 2D Ising and three-state Potts model. We found that in those systems small lattice sizes, up to 10×10, and modest amount of computer time are sufficient to determine the universal amplitudes with an accuracy of about one per cent.

There are two aspects that limit the accuracy: the statistical error in the values of the interfacial free energies at finite lattices, and the inaccuracy due to the extrapolation of these results to infinite lattice sizes. These effects work in opposite directions. The extrapolation improves if you study larger lattices, but the statistical error increases with lattice size. It requires much more computing time to reach the same statistics for larger lattices. To actually improve on the estimate of the universal amplitude you need to improve the statistics, otherwise the corrections to scaling to the universal amplitudes, since they scale with the lattice size, will drown in the statistical error. This implies that for a given amount of computer CPU there exists an optimal maximum lattice size. The question then arises whether this MC method is feasible with a modest amount of CPU time. This was the main purpose of our previous tests and also of the test reported here.

The Ising and three-state Potts model mentioned above, and also the transitions in the lattice gas model discussed here, are still simple enough that we can compare with results from the transfer matrix version of the FSS method, and also with other Monte Carlo methods. The strip widths used in transfer matrix calculations are typically smaller than the lattice sizes employed in MC calculations. The transfer matrix version of FSS is so successful, because it turns out that typically the asymptotic scaling regime, where only one or two corrections to scaling dominate, is reached quickly (in these relatively simple systems already at stripwidths of order $N < 18$).

To be able to extrapolate to infinite strip width, it is important that in transfer matrix calculations the interfacial free energies at finite N are known with *machine accuracy*. It is possible, however, to live with less accuracy. Our previous tests and also the one reported here confirm our expectation that, also in torus geometries, small lattice sizes up to 18×18 are sufficient to reach the the asymptotic scaling regime dominated by the leading corrections to scaling, and that with a modest amount of CPU computer time it is indeed possible to obtain enough statistical accuracy to make an extrapolation possible that leads to universal amplitudes with an accuracy at the one per cent level.

As mentioned above, the major reason for introducing this new MC method is that it is impossible to obtain the exact values of the largest eigenvalues of transfer matrices for large strip widths. Compared to the Monte Carlo renormalisation group (MCRG) method, our method has the advantage of being conceptionally simpler and is more versatile. For example, it does not lock you into a specific periodicity imposed by the cell spin structure required by the real-space renormalisation character of the MCRG method. This aspect is especially important in the study of the commensurate–incommensurate transitions.

In this paper we address three issues.

(i) We report the results of the test of our MC method on the $\sqrt{3} \times \sqrt{3}$ transition in the 2D Ising lattice gas, which requires a larger lattice and has a more complicated correction-to-scaling structure than in the Ising and three-state Potts model. We

show that with lattice sizes up to 18×18, we obtain the universal amplitude with an accuracy of 2% with a modest amount of computer time. We compare the numerical value of the universal amplitude with the exact analytical value for the non-chiral three-state Potts model which was determined recently by the authors. We find a good agreement within the numerical accuracy.

(ii) Our earlier MC algorithm for calculating the interfacial free energies, by means of periodic versus antiperiodic type boundary conditions, does not work for lattice gas models. Interfacial free energies for lattice gas models can be written in terms of free energy differences between systems with different sizes. We present the algorithm to calculate these interfacial free energy.

(iii) The $\sqrt{3} \times \sqrt{3}$ phase transition in the triangular lattice gas has been studied extensively in the past, e.g. by means of MC simulations (Landau 1983), and by means of transfer matrix calculations (Kinzel and Schick 1981). However, there are some interesting remaining aspects associated with the presence of chirality (Ostlund 1981, Huse 1981; for a review see den Nijs 1988) We address this issue. However, a systematic study of chirality effects in this model can be performed more efficiently using transfer matrices because the asymptotic scaling regime can be reached with the attainable maximum strip width $N = 18$.

Consider the triangular Ising antiferromagnet with Hamiltonian $\mathcal{H}$:

$$\mathcal{H} = \frac{K}{2} \sum_{<i,j>} \sigma_i \sigma_j + \frac{H}{2} \sum_i \sigma_i. \tag{1}$$

The first sum is over all nearest-neighbour pairs and $\sigma_i = \pm 1$ is the Ising spin at site i. As usual, the temperature $1/k_B T$ is absorbed in the coupling constants K and H. The nearest-neighbour coupling constant K is positive for antiferromagnets. Alternatively, the model can be represented as a lattice gas

$$\mathcal{H} = J \sum_{<i,j>} n_i n_j - \mu \sum_i n_i \tag{2}$$

with $\sigma_i = 2n_i - 1$, and $J = 2K$ and $\mu = 6K - H$. For $H > 0$, this model is suitable for the description of physisorbed monolayers like krypton or helium on graphite, because it exhibits a phase transition into an ordered $\sqrt{3} \times \sqrt{3}$ phase, see figure 1. The $\sqrt{3} \times \sqrt{3}$ ground state has threefold permutational degeneracy, and therefore was predicted to belong to the universality class of the three-state Potts model (Alexander 1975). Previous calculations (Kinzel and Schick 1981, Landau 1983) confirm that the critical exponents have the three-state Potts values. More recently it has been realised that the presence of chirality might change the nature of three-state Potts transitions (Huse and Fisher 1982). This model includes chirality. Numerical evidence from different models in the same universality class suggests that small amounts of chirality do not alter the critical exponents from three-state Potts values (for a review, see den Nijs 1988). It is *not* known yet whether the relation between universal finite-size scaling amplitudes on a torus and the critical exponents changes with the presence of chirality; most likely not. Our results for the universal amplitudes along with the previous results for the critical exponents provide evidence that the relation does not change with the presence of chirality.

Figure 2 shows the phase diagram obtained by Kinzel and Schick (1981). We limit our study to the line $2\mu = 3J$, where chirality almost vanishes. Along that line

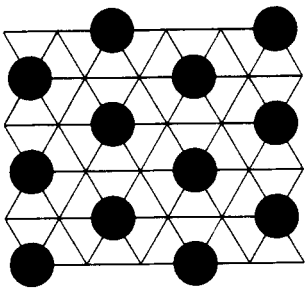

Figure 1. A $\sqrt{3} \times \sqrt{3}$ phase. Full circles represent gas atoms (or up spins) residing on lattice sites.

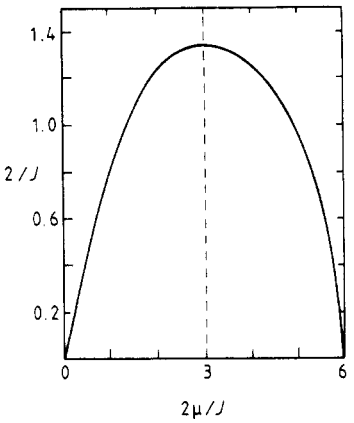

Figure 2. The phase diagram for the triangular Ising lattice gas. Taken from Kinzel and Schick (1981). We run Monte Carlo simulations along the $2\mu = 3J$ line (broken line).

chirality is completely absent at zero temperature. As we will see, chirality arises at finite temperatures because of a difference in intersection energies between the so-called clockwise and anticlockwise domain walls.

First, notice that the energy of a vacancy in the $\sqrt{3} \times \sqrt{3}$ state and that of an interstitial are the same at $2\mu = 3J$, i.e. $E(v) = \mu$ and $E(i) = -\mu + 3J$. This symmetry extends to the domain wall excitations. Label the three equivalent ground states by $\theta = 2\pi i/3$ with $i = 0, 1$, and 2. There are two topologically different types of domain walls. A domain wall with state i to the left and state $i + 1$ (mod 3) to the right is called a *clockwise* domain wall, and a wall with state i to the right and $i + 1$ to the left an *anticlockwise* interface. Chirality is associated with a (free) energy difference between these walls.

There are several possible microscopic arrangents to form walls. Walls with a local density higher than that of the commensurate ground states are called *heavy* or *superheavy* walls, while walls with a lower density than the commensurate density are referred to as *light* walls (for a general review on this topic see den Nijs 1988). Figures 3(*a*)–(*d*) show the elementary versions of each type: a heavy clockwise (HC) wall, a light clockwise (LC) wall, a superheavy anticlockwise (SA) wall, and a light anticlockwise (LA) wall. The excitation energies per $\sqrt{3}$ distance for these wall types,

when they are straight and do not meander, are easy to determine (see figure 4):

$$\begin{aligned} E(HC) &= -\mu/3 + J \qquad & E(LC) &= +2\mu/3 \\ E(SA) &= -2\mu/3 + 2J \qquad & E(LA) &= +\mu/3. \end{aligned} \tag{3}$$

In the hard hexagon model limit, $\mu \simeq 0$ (Baxter 1980), the light walls, LC and LA, dominate. In the opposite limit, close to zero magnetic field $H \simeq 0$ ($\mu \simeq 3J$), the (super) heavy walls, HC and SA, dominate. Close to $2\mu = 3J$ the HC and LA walls are the dominant microscopic configurations. Moreover, at $2\mu = 3J$ the difference in energy between clockwise and anticlockwise walls, i.e. chirality, vanishes entirely. The wall energies, and also the energies of vacancies and interstitials, are symmetric under reflection with respect to this point $2\mu = 3J$: $E(HC) \leftrightarrow E(LA)$, $E(LC) \leftrightarrow E(SA)$, and $E(v) \leftrightarrow E(i)$.

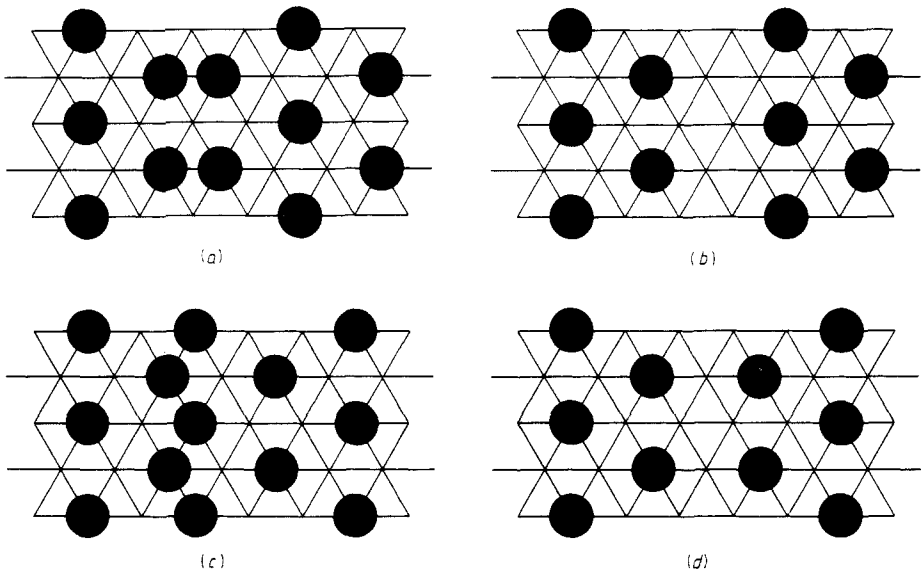

Figure 3. Interfaces in the triangular Ising lattice gas. (*a*) a heavy clockwise (HC) wall. (*b*) a light clockwise (LC)wall. (*c*) a superheavy anticlockwise (SA) wall. (*d*) a light anticlockwise (LA) wall.

This symmetry extends to the elementary excitations in the walls. Meander excitations do not break this symmetry. It is easy to check that the point-defect energies associated with a kink in the wall, i.e. turns of 60° (a HC wall transforms into a LA wall) and also turns over 120° (each wall type remains unchanged), are equal to zero in this model. The chiral symmetry does not get broken until one considers the core energies of intersections: an intersection where three HC walls meet (under 120°) costs an energy $E_{\rm int}(HC) = \mu/2$ while an intersection of three LA walls costs an energy $E_{\rm int}(LA) = -\mu/6$. It is slightly more complicated than that. The core energy can be lowered by removing one particle from the core, $E_{\rm int}(HC) = \mu/6 - \ln 3$ (removing two particles does not help).

This means that at finite temperatures the free energy of clockwise walls is larger than that of anticlockwise walls. But the degree of difference may be very small because there may be few excitations of the intersections when two types of domain

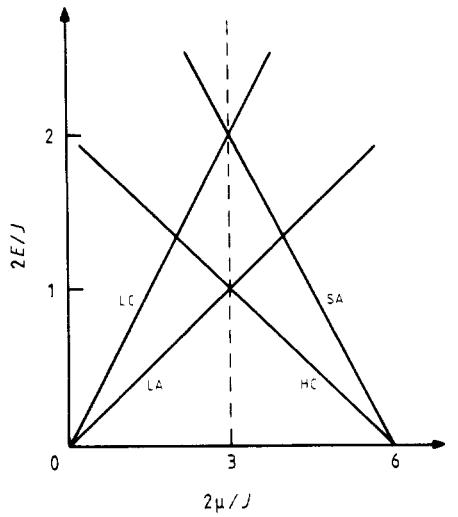

Figure 4. The excitation energies E for the interfaces.

walls are almost indistinguishable. So the line of zero chirality must bend slightly to the right in figure 2 ($2\mu > 3J$).

We now turn to the question of how to calculate these interfacial free energies in finite systems by Monte Carlo simulations. The conventional method of calculating the interfacial free energy in, e.g., the ferromagnetic Ising model is to compare a system with periodic and antiperiodic boundary conditions (Park and den Nijs 1988, 1989). The antiperiodic boundary condition imposes a Bloch wall in the system, and therefore the free energy difference between the two systems is equal to the Bloch wall free energy. This does not work for the lattice-gas model due to the presence of the magnetic field. The magnetic field destroys the gauge invariance of the seam (the boundary with modified interactions to impose the interface). The free energy difference between systems with these two boundary conditions includes not only the free energy of the interface but also the free energy of the seam. Moreover, pinning behaviour of the interface with respect to the seam adds another contribution to the free energy difference. Such effects have been discussed in detail recently by Blöte and den Nijs (1988). So it is useful to find a way to force an interface into the system without seams.

Consider a $N_x \times N_y$ triangular lattice with periodic boundary conditions in both the horizontal (x) and the vertical (y) directions (figure 5). In order to create a $\sqrt{3}\times\sqrt{3}$ phase without frustrations, N_x must be a multiple of three, i.e. $N_x = 3n_x$ where n_x is a positive integer. In addition, N_y must be a multiple of six, i.e. $N_y = 6n_y$, because this lattice is periodic in every two rows of triangles in the vertical direction. For example, a 6×6 lattice can accommodate a $\sqrt{3}\times\sqrt{3}$ configuration without frustrations, see figure 5(a). Clockwise (anticlockwise) interfaces in the vertical direction can be imposed by increasing (decreasing) the number of triangles in the horizontal direction N_x, by one, i.e. $N_x \rightarrow N_x \pm 1$, see figure 5($b$), ($c$). A lattice with $N_x = 3n_x + 1$ should contain a clockwise wall in the vertical direction and a lattice with $N_x = 3n_x - 1$ an anticlockwise wall.

The horizontal length of the lattice $L_x = N_x d$ (where d is the lattice constant) and the vertical length $L_y = (\sqrt{3}/2)N_y d$. So the aspect ratio $s = L_x/L_y = (2/\sqrt{3})N_x/N_y$.

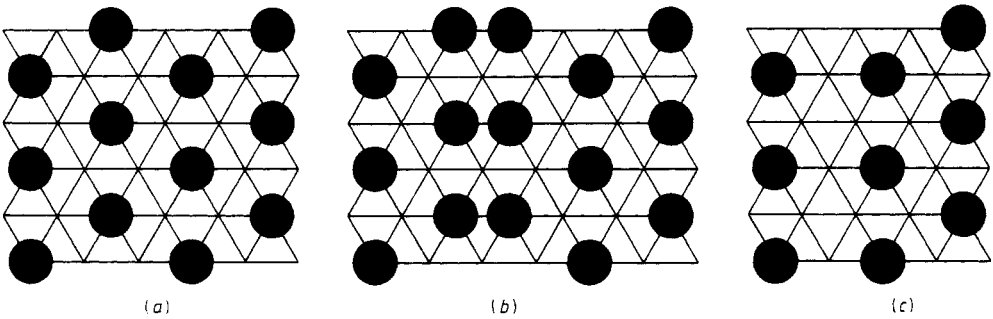

Figure 5. (*a*) A $\sqrt{3} \times \sqrt{3}$ configuration on a 6×6 lattice with periodic boundary conditions. (*b*) A clockwise interface in the vertical direction on a 7×6 lattice, imposed by periodic boundary conditions. (*c*) An anticlockwise interface in the vertical direction on a 5×6 lattice, imposed by periodic boundary conditions.

The interfacial free energies per unit length of clockwise and anticlockwise walls, η_+ and η_-, are given as

$$\eta_\pm(N_x, N_y) = [F_\pm(N_x, N_y) - F_0(N_x, N_y)]/L_y \tag{4}$$

where F_+, F_0, and F_- represent the total free energy of the system with $N_x = +1$, 0, and -1 (mod 3) respectively. Strictly speaking, these free energies can not be defined for the same value of N_x. Therefore we need to interpolate. The free energy $F_\pm$ at $N_x = 0$ (mod 3) is defined as

$$F_\pm(N_x, N_y) = \tfrac{2}{3}F_\pm(N_x \pm 1, N_y) + \tfrac{1}{3}F_\pm(N_x \mp 2, N_y). \tag{5}$$

This type of interpolation creates an artificial correction to scaling, but only of order N_x^{-3}. Similarly, we interpolate

$$\begin{aligned} F_0(N_x \pm 1, N_y) &= \tfrac{2}{3}F_0(N_x, N_y) + \tfrac{1}{3}F_0(N_x \pm 3, N_y) \\ F_\pm(N_x \mp 1, N_y) &= \tfrac{2}{3}F_\pm(N_x \mp 2, N_y) + \tfrac{1}{3}F_\pm(N_x \pm 1, N_y) \end{aligned} \tag{6}$$

where $N_x = 0$ (mod 3).

The interfacial free energies $\eta_\pm(N_x, N_y)$ at $N_x = 0$ (mod 3) are now rewritten as

$$\eta_\pm(N_x, N_y) = [\tfrac{2}{3}F_\pm(N_x \pm 1, N_y) + \tfrac{1}{3}F_\pm(N_x \mp 2, N_y) - F_0(N_x, N_y)]/L_y. \tag{7}$$

The interfacial free energies $\eta_\pm$ at $N_x = \pm 1$ (mod 3) can be rewritten similarly.

The interfacial free energy η is finite in the ordered phase, vanishes in the disordered phase, and scales at criticality (Nightingale 1976, 1982, Privman and Fisher 1984) as

$$\eta(L_x, L_y) = L_x^{-1}(A(s) + B(s)L_x^{y_{ir}} + \cdots) \tag{8}$$

where $s = L_x/L_y$ the aspect ratio and $y_{ir} < 0$ the irrelevant exponent. The amplitude $A(s)$ is universal and varies continuously with the aspect ratio s (Park and den Nijs 1988), while the amplitude $B(s)$ is non-universal.

In Monte Carlo simulations, it is difficult to obtain the free energy directly, but the free energy difference $\Delta F = F - F'$ between two systems with similar Hamiltonians

$\mathcal{H}$ and $\mathcal{H}'$ can be written in terms of ensemble averages (Bennett 1976, Park and den Nijs 1989) as

$$\langle f(\mathcal{H}' - \mathcal{H} + \Delta F)\rangle_{\mathcal{H}} = \langle f(\mathcal{H} - \mathcal{H}' - \Delta F)\rangle_{\mathcal{H}'} \tag{9}$$

with $f(x) = 1/(1+\mathrm{e}^x)$, the Fermi function which is the optimal choice according to Bennett (1976). In our earlier tests for the Ising and three-state Potts model, the two systems were of the same size but had different boundary conditions. Now we compare systems with the same boundary conditions, but with different sizes. We calculate the free energy difference between two systems where the horizontal sizes N_x differ by one, i.e. $\Delta F(N_x - \frac{1}{2}, N_y) \equiv F(N_x, N_y) - F(N_x - 1, N_y)$. All interfacial free energies can be rewritten in terms of these free energy differences ΔF, e.g. $\eta_{\pm}(N_x, N_y)$ at $N_x = 0$ (mod 3) in (7) is given as

$$\begin{aligned}\eta_{\pm}(N_x, N_y) = [&\pm\tfrac{2}{3}\Delta F(N_x \pm \tfrac{1}{2}, N_y) \mp \tfrac{1}{3}\Delta F(N_x \mp \tfrac{1}{2}, N_y) \\ &\mp \tfrac{1}{3}\Delta F(N_x \mp \tfrac{3}{2}, N_y)]/L_y.\end{aligned} \tag{10}$$

Similarly, $\eta_{\pm}$ at $N_x = \pm 1$ (mod 3) can be obtained in terms of ΔF.

To calculate the free energy difference $\Delta F(N_x - \frac{1}{2}, N_y)$ between systems of different size (N_x, N_y) and $(N_x - 1, N_y)$, consider an intermediate system with size (N_x, N_y) by adding a column of *ghost* spins in the vertical (y) direction to the system with the size $(N_x - 1, N_y)$ (see figure 6). All the coupling constants associated with these ghost spins are set to be zero, so they do not couple with any other spin or the magnetic field. The total free energy of this intermediate system, F_{I}, is the free energy of the original system minus the entropy of ghost spins; $F_{\mathrm{I}}(N_x, N_y) = F(N_x - 1, N_y) - N_y \ln 2$. The free energy difference $\Delta F(N_x - \frac{1}{2}, N_y)$ can then be obtained by solving the modified equation from (9) as

$$\langle f(\mathcal{H}_{\mathrm{I}} - \mathcal{H} + \Delta F + N_y \ln 2)\rangle_{\mathcal{H}} = \langle f(\mathcal{H} - \mathcal{H}_{\mathrm{I}} - \Delta F - N_y \ln 2)\rangle_{\mathcal{H}_{\mathrm{I}}} \tag{11}$$

where $\mathcal{H}_{\mathrm{I}}$ is the Hamiltonian of the intermediate system of size (N_x, N_y). In practice, we run two MC simulations with the Hamiltonian $\mathcal{H}$ (1) on a triangular lattice with two different sizes, $(N_x - 1, N_y)$ and (N_x, N_y). The configurations of the intermediate system $\mathcal{H}_{\mathrm{I}}$ with size (N_x, N_y) are obtained from the configurations of the system $\mathcal{H}$ with size $(N_x - 1, N_y)$ by adding a column of randomly generated ghost spins. During both simulations, we store the probability distribution $P(\Delta\mathcal{H})$, with $\Delta\mathcal{H} = \mathcal{H} - \mathcal{H}_{\mathrm{I}}$. Afterwards ΔF follows easily by solving the equation

$$\sum_h P_{\mathcal{H}}(h) f(\Delta F + N_y \ln 2 - h) = \sum_h P_{\mathcal{H}_{\mathrm{I}}}(h) f(h - \Delta F - N_y \ln 2). \tag{12}$$

The configurations of the system with size (N_x, N_y) are used for the calculation of not only $\Delta F(N_x - \frac{1}{2}, N_y)$ but also $\Delta F(N_x + \frac{1}{2}, N_y)$ by supplying configurations of the intermediate system with size $(N_x + 1, N_y)$. Notice that one can also obtain accurate values of the bulk free energies by extrapolating ΔF ($\lim_{N_y \to \infty} \Delta F/N_y = f$: the bulk free energy density per site).

We consider lattices with vertical sizes $6n$ and horizontal sizes $6n + i$ ($n = 1, 2, 3$ and $i = 0, \pm 1, \pm 2, \pm 3$). We use 10^6 MC steps per spin (MCS) for each lattice at a given temperature. So the free energy differences ΔF are obtained for $N_x = 6n \pm 5/2, 6n \pm 3/2$, and $6n \pm 1/2$ and $N_y = 6n$. From (10), both the clockwise and anticlockwise

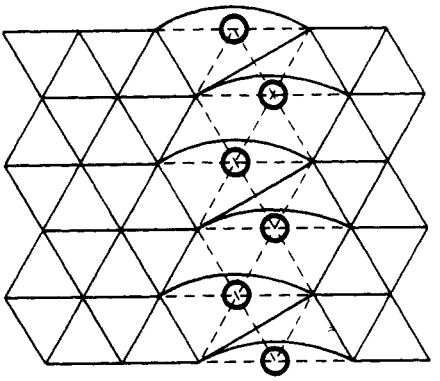

Figure 6. Construction of the intermediate system with size (N_x, N_y) from the system with size $(N_x - 1, N_y)$ by adding a column of ghost spins (denoted by open circles). Line segments between spins denote the ordinary couplings with strength J and broken line segments the zero couplings.

interfacial free energies, $\eta_\pm$, are calculated for $N_x = 6n \pm 1$ and $6n$ and $N_y = 6n$ $(n = 1, 2, 3)$. In the infinite-lattice limit, we have

$$N_x \eta_\pm(N_x, N_y) = [(N_x + 1)\eta_\pm(N_x + 1, N_y) + (N_x - 1)\eta_\pm(N_x - 1, N_y)]/2 \tag{13}$$

where we use the scaling relation of the interfacial free energies, see (8). The aspect ratio of this system $(N_x = N_y)$ is equal to $s = L_x/L_y = 2/\sqrt{3}$. The exact value of the universal amplitude for the non-chiral three-state Potts model is $A(s = 2/\sqrt{3}) = 1.203291\cdots$ (Park and den Nijs 1988). Note that an accuracy of about 1–2% is sufficient to distinguish universality classes; for example, the universal amplitude for the Ising model at this value of aspect ratio is $0.989\,556\cdots$.

First we run standard Monte Carlo simulations at two temperatures: $\exp(-J/2) = 0.225$ and 0.226 $(2\mu = 3J)$. The results for $L_x\eta_\pm$ are plotted against N^{-1}, see figure 7. From the curvature of these curves, we estimate the critical temperature $\exp(-J_c/2) = 0.2257 \pm 0.0001$. This value agrees very well with the results from the transfer matrix calculations (Kinzel and Schick 1981). Then we run Monte Carlo simulations at this critical temperature. The result is shown in figure 7.

The results for the univeral FSS amplitudes of the clockwise and anticlockwise wall free energies extrapolate to the same value, within the numerical accuracy, identical to the exact value for the non-chiral three-state Potts model: $A_\pm(s = 2/\sqrt{3}) = 1.22 \pm 0.02$ (see table 1). As a check, we carried out a simulation at $\exp(-J/2) = 0.2258$, and found no noticeable change in the value of the universal amplitude within statistical errors.

The most important result is that we are able to determine the universal amplitude with an accuracy of about 2%, with relatively small lattice sizes and modest amounts of CPU. Within this accuracy, the transition along the $2\mu = 3J$ line has the same universal amplitude as in the non-chiral three-state Potts universality class. If one employs more sophisticated simulation algorithms such as the Swendsen–Wang algorithm (Swendsen and Wang 1987, Wang *et al* 1989) and recently developed data-analysis techniques such as the (multi-) histogram method (Ferrenberg and Swendsen 1988, 1989), then the accuracy for the universal amplitudes should improve significantly (we learned of these techniques after the completion of our standard Monte Carlo simulations). These rapidly developing techniques in Monte Carlo simulations will guarantee a good

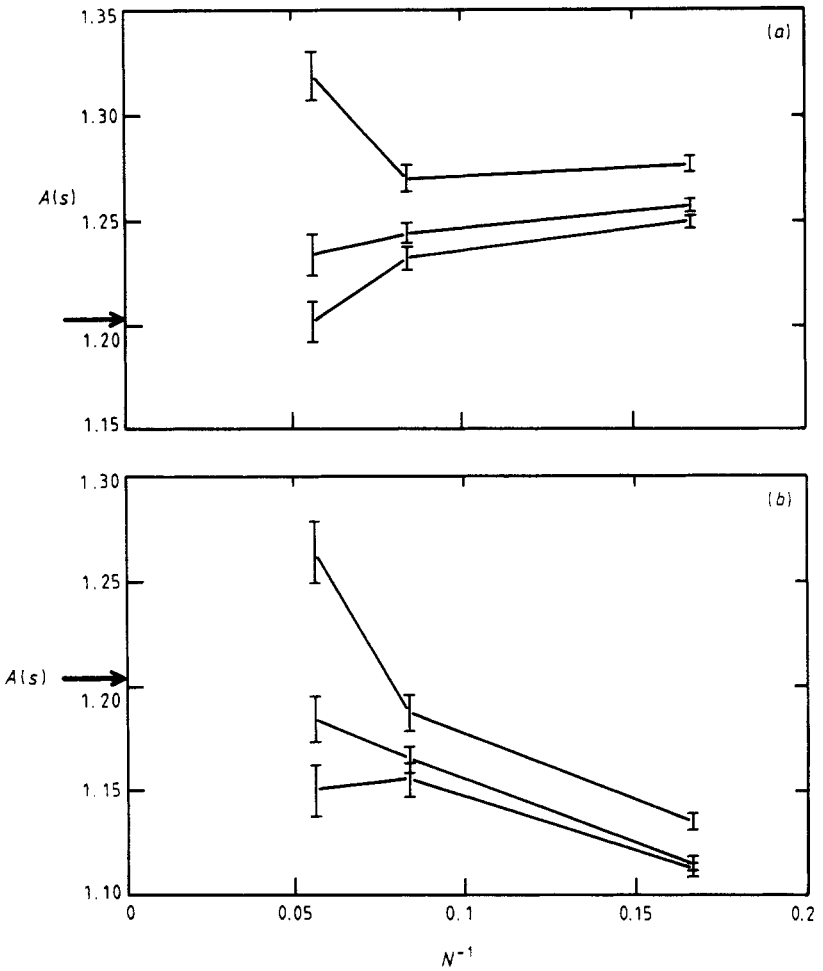

Figure 7. Finite-size scaling behaviour of (*a*) the clockwise and (*b*) the anticlockwise interfaces at several different temperatures $\exp(-J/2) = 0.2250$, 0.2257, and 0.2260. The arrow indicates the exact value of the universal amplitude $A(s = 2/\sqrt{3})$ for the non-chiral three-state Potts model.

Table 1. The universal amplitudes $A_{\pm}(s = 2/\sqrt{3})$ of the triangular Ising lattice gas at the temperature $\exp(-J/2) = 0.2257$ (the estimated critical temperature) and $2\mu = 3J$. The value in the last row is an extrapolation to the thermodynamic limit ($N_x = \infty$) of the Monte Carlo data.

N_x	$A_+(s)$	$A_-(s)$
6	1.2568 ± 0.0037	1.1149 ± 0.0032
12	1.2443 ± 0.0047	1.1642 ± 0.0071
18	1.2339 ± 0.0105	1.1898 ± 0.0121
∞	1.22 ± 0.02	

numerical accuracy in measuring the universal amplitudes of more complex systems where larger lattice sizes are needed.

Moreover, our results shed some light on the physics of the triangular Ising lattice

gas. Although absent at zero temperature, chirality is present at finite temperatures along the line $2\mu = 3J$. The values of clockwise and anticlockwise interfacial free energies at finite sizes are not the same. In accordance with the discussion at the beginning of this paper, the anticlockwise walls have a lower free energy. But asymptotically, i.e. at the critical point in the thermodynamic limit the difference vanishes and we obtain the same universal leading FSS amplitudes. In a case like this we expect that the clockwise and anticlockwise interfaces have the same leading irrelevant exponents $y_{T,2} = -4/5$ and $y_{CH} = -1$ (den Nijs 1984). Indeed, the curves in figure 7 are consistent with almost straight lines. The difference in the slopes manifests the presence of the chirality. The corrections to scaling due to the leading irrelevant thermal operator ($y_{T,2}$) and the leading chiral operator (y_{CH}) can be distinguished in principle by adding or substracting the two interfacial free energies. The amplitudes of the corrections to scaling associated with $y_{T,2}$ must be the same. With statistical errors as much as 1% for 18×18 lattices, it is doubtful to distinguish such details into the numerical results. However, the data are consistent with the theory.

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References

Alexander S 1975 *Phys. Lett.* **54A** 353
Baxter R J 1980 *J. Phys. A: Math. Gen.* **13** L61
Bennett C H 1976 *J. Comp. Phys.* **22** 245
Blöte H W J and den Nijs M 1988 *Phys. Rev.* B **37** 1766
Blöte H W J and Nightingale M P 1985 *Physica* **134A** 274
Cardy J L 1984 *J. Phys. A: Math. Gen.* **17** L385
den Nijs M 1984 *J. Phys. A: Math. Gen.* **17** L295
—— 1988 *Phase Transitions and Critical Phenomena* vol 12, ed C Domb and J L Lebowitz (New York: Academic) ch 2
Ferrenberg A M and Swendsen R H 1988 *Phys. Rev. Lett.* **61** 2635
—— 1989 *Phys. Rev. Lett.* **63** 1195
Huse D A 1981 *Phys. Rev.* B **24** 5180
Huse D A and Fisher M E 1982 *Phys. Rev. Lett.* **49** 793
Kinzel W and Schick M 1981 *Phys. Rev.* B **23** 3435
Landau D P 1983 *Phys. Rev.* B **27** 5604
Luck J M 1982 *J. Phys. A: Math. Gen.* **15** L169
Nightingale M P 1976 *Physica* **83A** 561
—— 1982 *J. Appl. Phys.* **53** 7927
Ostlund S 1981 *Phys. Rev.* B **24** 398
Park H and den Nijs M 1988 *Phys. Rev.* B **38** 565
—— 1989 *J. Phys. A: Math. Gen.* **22** 3663
Park H, Riedel E K and den Nijs M 1986 *Ann. Phys., NY* **172** 419
Park H and Widom M 1989 *Phys. Rev. Lett.* **63** 1193
—— 1990 *Phys. Rev. Lett.* **64** 1076
Privman V and Fisher M E 1984 *Phys. Rev.* B **30** 322
Saleur H 1987 *J. Phys. A: Math. Gen.* **20** L1127
Swendsen R H and Wang J S 1987 *Phys. Rev. Lett.* **58** 86
Wang J S, Swendsen R H and Kotecký R 1989 Phys. Rev. Lett. **63** 109