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LETTER TO THE EDITOR

Correlation length in Ising strips with free and fixed boundary conditions

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Abstract. The correlation length of boundary spins in the Ising model, defined on strips of triangular lattice with free boundary conditions, is determined with an efficient numerical procedure based on the star-triangle transformation. In the case of isotropic critical interactions, the extrapolated amplitude of the correlation length is in excellent agreement with the value $2/(\pi\eta_{\parallel})$ predicted by conformal invariance. An analytical formula for the amplitude in strips with anisotropic interactions is proposed. Fixing the spins on one edge reduces the amplitude of the correlation length on the other edge by a factor $\frac{1}{2}$. The convergence of phenomenological renormalisation with free boundary conditions is studied.

According to the theory of finite-size scaling (Barber 1983), the longitudinal spin-spin correlation length $\xi(T, L)$ in a spin system, defined on a two-dimensional strip of finite width L and infinite length, varies as

$$\xi(T_c, L) \approx AL, \qquad L \to \infty \tag{1}$$

at criticality, where the amplitude A is a constant. In a recent letter Cardy (1984) showed that conformal invariance of the correlations in systems with isotropic interactions implies the universal values

$$A = (\pi\eta)^{-1}, \qquad \text{periodic boundary conditions,} \tag{2a}$$

$$= 2(\pi\eta_{\parallel})^{-1}, \qquad \text{free boundary conditions,} \tag{2b}$$

where η and $\eta_{\parallel}$ are the standard bulk (Patashinskii and Pokrovskii 1979) and surface (Binder 1983) critical exponents. Exact calculations and numerical studies (Derrida and de Seze 1982, Nightingale and Blöte 1983) have indicated that equation (2a) is satisfied in a variety of models. In this letter we report results confirming (2b) in the Ising model.

We have considered strips of Ising spins with finite width and infinite length. The strips have a triangular lattice structure and are made up of $N+1$ columns of spins, as shown for $N=2$ in figure 1. The width L in lattice constants is $L=\sqrt{3}\,N/2$. The couplings in the three principal directions of triangular lattice are denoted by K_1, K_2, K_3, with the K_1 bonds oriented parallel to the edges of the strip, as in figure 1.

With a numerical method based on the star-triangle transformation, we have calculated the correlation length ξ_N of spins on the left edge, with free boundary conditions on the left edge and with either free or fixed boundary conditions on the

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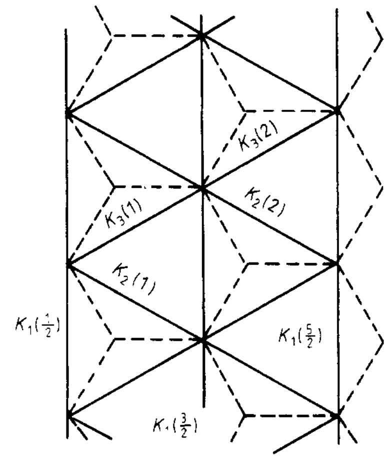

Figure 1. Strip with three layers ($N=2$). The full lines indicate the original triangular lattice and the broken lines the intermediate hexagonal lattice.

right edge. In the fixed-boundary calculations the spins on the right edge were 'frozen' by an infinite edge coupling. The amplitude A was determined by extrapolation from numerical results for values of N up to 100. With a finite field applied to the spins on the right edge, the extrapolation yields a result indistinguishable from the extrapolated result with 'frozen' couplings or an initially infinite field.

On the basis of our numerical results (which are presented below), we propose the formulae

$$\lim_{N\to\infty}\frac{\xi_N}{N} = (2/\pi)(\sinh 2K_2+\sinh 2K_3)^{-1}, \qquad \text{free boundary conditions on right edge} \tag{3a}$$

$$= (1/\pi)(\sinh 2K_2+\sinh 2K_3)^{-1}, \qquad \text{fixed boundary conditions on right edge} \tag{3b}$$

where the couplings satisfy the Houtappel (1950) criticality condition

$$\sinh 2K_1 \sinh 2K_2 + \sinh 2K_2 \sinh 2K_3 + \sinh 2K_3 \sinh 2K_1 = 1. \tag{4}$$

We are unaware of a rigorous derivation of equations (3). The factors $(\sinh 2K_2+\sinh 2K_3)^{-1}$ follow from an intuitive argument (Barber *et al* 1984) in which the lattice is rescaled so that the bulk correlation length diverges isotropically. Equations (3) resemble the exact result

$$\lim_{N\to\infty}\frac{\xi_N}{N} = \frac{4}{\pi}(\sinh 2K_2)^{-1}, \qquad \text{square lattice with periodic boundary conditions} \tag{5}$$

of Nightingale and Blöte (1983) for the square lattice with periodic boundary conditions.

Since $\eta_\parallel = 1$ for the two-dimensional Ising model (McCoy and Wu 1973), and since $\sinh 2K = 1/\sqrt{3}$ and $L=\sqrt{3}\,N/2$ for a triangular lattice with isotropic interactions, equation (3a) is consistent with prediction (2b). There is also complete consistency in the special cases $K_1=0$, $K_2=K_3$; $K_2=0$, $K_1=K_3$; $K_3=0$, $K_1=K_2$ in which a square lattice with isotropic interactions is obtained. (When the triangular lattice is distorted so that the square lattice has equal and perpendicular bond lengths, $L = N/2$ in the first case and $L = N$ in the second and third cases; in (3) and (5) the correlation length is specified in units of the lattice constant parallel to the edges.)

We now briefly discuss the method used to calculate ξ_N. With modest computing times it yields results for strip widths far larger than the largest considered thus far with numerical transfer-matrix methods (Nightingale 1982, Barber 1983). The method utilises an exact mapping, based on the star–triangle transformation (Syozi 1972), that replaces a strip with couplings $K_1(m-\frac{1}{2}, n)$, $K_2(m, n)$, $K_3(m, n)$ by a similar strip with transformed couplings $K_1(m-\frac{1}{2}, n+1)$, $K_2(m, n+1)$, $K_3(m, n+1)$. The index $m = 1, 2, \ldots$ labels the couplings in order of increasing distance from the left edge, there being $N+1$ couplings K_1 and N couplings K_2 and K_3, as in figure 1. The mapping is carried out by replacing all right-pointing triangles of the strip by stars to obtain an intermediate hexagonal lattice (see figure 1) and then eliminating the left-pointing stars to obtain a strip of triangular lattice, with transformed couplings and with the same width† as the original strip. This mapping has been used to study surface critical behaviour in the semi-infinite Ising model (Hilhorst and van Leeuwen 1981, Burkhardt and Guim 1984, Burkhardt *et al* 1984), and we refer to these papers for details.

The explicit form of the transformation from the nth to the $n+1$st coupling constants in the subspace $K_2(m, n) = K_3(m, n)$ is given in Burkhardt *et al* (1984). The generalisation to $K_2 \neq K_3$ is straightforward, and a magnetic field applied to the spins on the edge may also be included. Some convenient variables that simplify the star–triangle transformation are discussed in Syozi (1972).

The boundary magnetisation $m_1(n)$ and pair correlation function $g_{\|}(r, n)$ of boundary spins transform under the mapping according to

$$m_1(n) = \{1 - \exp[-4K_1(\tfrac{1}{2}, n+1)]\}^{1/2} m_1(n+1) \tag{6a}$$

$$g_{\|}(r, n) = \tfrac{1}{4}\{1 - \exp[-4K_1(\tfrac{1}{2}, n+1)]\}[g_{\|}(r+1, n+1) + 2g_{\|}(r, n+1) + g_{\|}(r-1, n+1)], \qquad r \geqslant 1. \tag{6b}$$

The magnetisation and pair correlation function of the initial system are determined by the sequence of edge couplings $K_1(\frac{1}{2}, n)$ according to (Hilhorst and van Leeuwen 1981, Burkhardt *et al* 1984)

$$m_1(0) = \pm[f(\infty)]^{1/2} \tag{7a}$$

$$g_{\|}(r, 0) = \sum_{n=1}^{\infty} 4^{-n} \frac{r}{n} \binom{2n}{n+r} f(n)[1 - m_1^2(n)] \tag{7b}$$

$$f(n) = \prod_{j=1}^{n} \{1 - \exp[-4K_1(\tfrac{1}{2}, j)]\}. \tag{7c}$$

When the mapping is iterated with homogeneous critical initial couplings (either isotropic or anisotropic) and with free boundary conditions on both edges, $\exp[-4K_1(\frac{1}{2}, n)]$ varies as $(2n)^{-1}$ for $1 \ll n \ll N^2$ and approaches a constant value for $n \gg N^2$. This behaviour can be understood from an analytic solution of the differential

† With the star–triangle transformation, one can also map a triangular lattice in the form of a triangle onto a similar system with modified couplings and fewer spins. This type of transformation has been utilised in the exact differential renormalisation of the Ising model (Hilhorst *et al* 1979) and in the computation of corner critical exponents (Barber *et al* 1984). In the application to strips considered in this letter, there is no reduction in the number of spins.

flow equations (Burkhardt *et al* 1984) in the strip geometry. It follows from equations (7) that $m_1(0)=0$, as expected, and that $g_\parallel(r,0)$ decays exponentially with correlation length

$$\xi_N = \tfrac{1}{2}|\ln\{1-\exp[-4K_1(\tfrac{1}{2},\infty)]\}|^{-1/2} \qquad \text{free boundary conditions on right edge.} \tag{8}$$

With fixed boundary conditions on the right edge (an infinite edge coupling or a finite field), $\exp[-4K_1(\frac{1}{2},n)]$ again varies as $(2n)^{-1}$ for $1 \ll n \ll N^2$. For $n \gg N^2$, $K_2(1,n)$ and $K_3(1,n)$ approach a limiting value $K_2(1,\infty)=K_3(1,\infty)$. (After N iterations $K_2(m,n)=K_3(m,n)$ for $m=1,2,\ldots,N$.) From the transformation

$$\exp[-4K_1(\tfrac{1}{2},n+1)] = \exp[-4K_1(\tfrac{1}{2},n)]/\cosh^2 2K_2(1,n) \tag{9}$$

for the edge couplings (Burkhardt *et al* 1984), one sees that $\exp[-4K_1(\frac{1}{2},n)] \sim [\cosh 2K_2(1,\infty)]^{-2n}$ for $n \gg N^2$. From (7*a*) it follows that $m_1(0)$ varies as $N^{-1/2}$ for large N, a result in agreement with the scaling prediction $m_1 \sim N^{-\beta_1/\nu}$ (Fisher and de Gennes 1978) and with previous exact work on the two-dimensional Ising model (Au-Yang and Fisher 1980). From equations (7*b*) and (7*c*), one derives

$$\xi_N = \tfrac{1}{2}\{\ln[\cosh^2 2K_2(1,\infty)]\}^{-1/2} \qquad \text{fixed boundary conditions on right edge} \tag{10}$$

for the correlation length.

Our numerical procedure for determining ξ_N was extremely simple. We iterated the mapping of the coupling constants until $K_1(\frac{1}{2},n)$ or $K_2(1,n)$ remained constant to within 1 part in 10^9 per iteration (about $3N^2$ iterations are required) and then calculated ξ_N with equation (8) or (10), respectively. Determining ξ_N for a strip with $N=100$ on a DEC-10 computer required about three minutes of computer time.

Figures 2 and 3 show ξ_N/N as a function of N^{-1} at criticality for $N=6$, 8, 12, 16, 20, 28, 40, 56, 100 with free and fixed (or finite-field) boundary conditions on the right edge, respectively. Several different sets of critical couplings are considered. In every case the results extrapolate linearly to values indistinguishable from the encircled points, which give the predictions of equations (3*a*) and (3*b*). The beautiful agreement leads us to believe that (3*a*) and (3*b*) are exact. Note in figure 3 that the results for fixed-spin (infinite field) and finite-field boundary conditions on the right edge extrapolate to the same point. (The finite field increases without bound on iteration of the mapping.) Some of the results shown in figure 2 are listed in table 1.

The finite-size scaling method known as phenomenological renormalisation (Nightingale 1982, Barber 1983) has proved to be an extremely reliable method for determining the bulk critical properties of low-dimensional systems. The convergence with increasing strip width of the estimates furnished by phenomenological renormalisation toward exact bulk results has been studied numerically (Nightingale 1976) and analytically (Derrida and de Seze 1982) in Ising strips with periodic boundary conditions. Equation (2*b*) provides a way of determining the surface critical exponent $\eta_\parallel$ using phenomenological renormalisation with free boundary conditions. We now present numerical information we have obtained on the convergence of phenomenological renormalisation with free boundary conditions in Ising strips.

Comparing strips of N and $N-1$ layers and considering only the subspace $K_1 = K_2 = K_3 = K$ of isotropic interactions, we write the fundamental equation of phenomenological renormalisation in the form

$$\xi_{N-1}(K') = [(N-1)/N]\xi_N(K). \tag{11}$$

The fixed point $K^*(N)$ of equation (11) furnishes an estimate of the critical coupling.

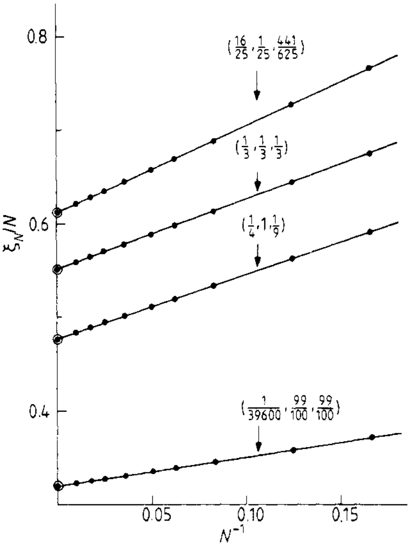

Figure 2. Calculated values of ξ_N/N with free boundary conditions for $N=6$, 8, 12, 16, 20, 28, 40, 56 and 100. The encircled points at $N=\infty$ are predictions of equation (3a). The numbers (S_1^2, S_2^2, S_3^2) specify the critical couplings, with $S_i=\sinh 2K_i$.

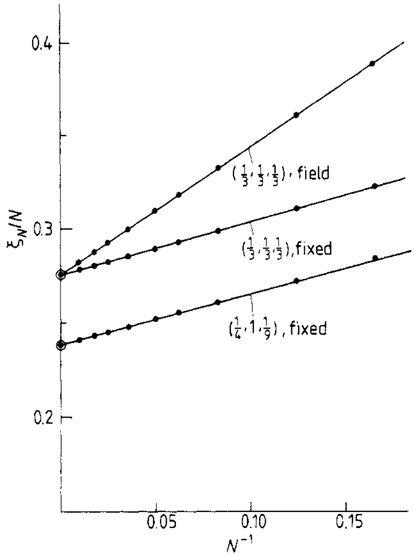

Figure 3. Calculated values of ξ_N/N with fixed boundary conditions for $N=6$, 8, 12, 20, 28, 40, 56 and 100. The sequences of points marked 'fixed' and 'field' were calculated with fixed (infinite-field) and finite-field ($\sinh^2 h=0.1$) boundary conditions on the right edge, respectively. The encircled points at $N=\infty$ are predictions of equation (3b). The numbers (S_1^2, S_2^2, S_3^2) specify the critical couplings, with $S_i=\sinh 2K_i$.

Table 1. Values of ξ_N/N at criticality for free boundary conditions; $S_i=\sinh 2K_i$. The entries for $N=\infty$ follow from equation (3a).

N	$S_1=S_2=S_3=1/\sqrt{3}$	$S_1=\frac{1}{2}, S_2=1, S_3=\frac{1}{3}$
6	0.6748	0.5913
8	0.6438	0.5626
12	0.6128	0.5341
16	0.5974	0.5198
20	0.5882	0.5113
28	0.5776	0.5016
40	0.5697	0.4944
56	0.5645	0.4895
100	0.5587	0.4842
⋮	⋮	⋮
∞	0.5513	0.4775

An estimate $y_t(N)$ for the thermal scaling index (Patashinskii and Pokrovskii 1979) is given by (Nightingale 1982)

$$y_t(N)=\frac{\ln[\xi'_N(K^*(N))/\xi'_{N-1}(K^*(N))]}{\ln[N/(N-1)]}-1 \tag{12}$$

where the primes denote differentiation with respect to the argument K. Finally we obtain an estimate $y_{h_1}(N)$ of the surface magnetic scaling index $y_{h_1} = d - 1 - \eta_{\parallel}/2$ (Binder 1983) from

$$y_{h_1}(N) = 1 - (\sqrt{3}/2\pi)[N/\xi_N(K^*(N))] \tag{13}$$

in accordance with equations (1) and (2*b*).

Our results for $K^*(N)$, $y_t(N)$, and $y_{h_1}(N)$ in strips of triangular lattice with free boundary conditions are compared with Nightingale's (1976) data for strips of square lattice with periodic boundary conditions in figures 4 and 5. As one might have expected, the convergence to the exact results is considerably faster in the case of periodic boundaries. According to the analytical results of Derrida and de Seze (1982), $K^*(\infty) - K^*(N) \sim N^{-3}$ and $y_t(\infty) - y_t(N) \sim N^{-2}$ for the square lattice with periodic boundary conditions in the large-N limit. Our numerical results for the triangular lattice with free boundaries are consistent with the asymptotic forms $K^*(\infty) - K^*(N) \sim N^{-2}$, $y_t(\infty) - y_t(N) \sim N^{-1}$, $y_{h_1}(\infty) - y_{h_1}(N) \sim N^{-1}$ derived analytically (Burkhardt and Guim 1985) for the square lattice with free boundaries in the extreme anisotropic or quantum-Hamiltonian limit.

Using the star-triangle method to calculate the correlation length ξ_N for strip widths up to $N = 100$, we have confirmed prediction (2*b*) in Ising strips with free boundaries, proposed a generalisation for anisotropic couplings, considered the effects of fixed boundary conditions, and studied the convergence of phenomenological renormalisation with free boundaries. Unfortunately, the star-triangle method for calculating ξ_N is only applicable to a few systems. The system must, of course, have a star-triangle transformation. In addition, thermal averages of the edge spins must transform as in (6*a*) and (6*b*), without generating more complicated correlation functions.

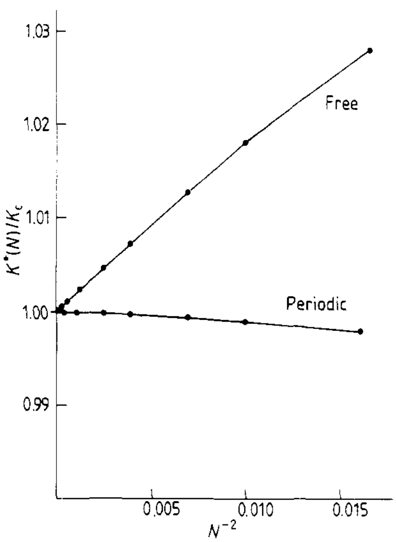

Figure 4. Estimates $K^*(N)$ of the bulk critical coupling K_c obtained with phenomenological renormalisation. 'Free' and 'periodic' label results for strips of triangular lattice with free boundary conditions and strips of square lattice with periodic boundary conditions, respectively.

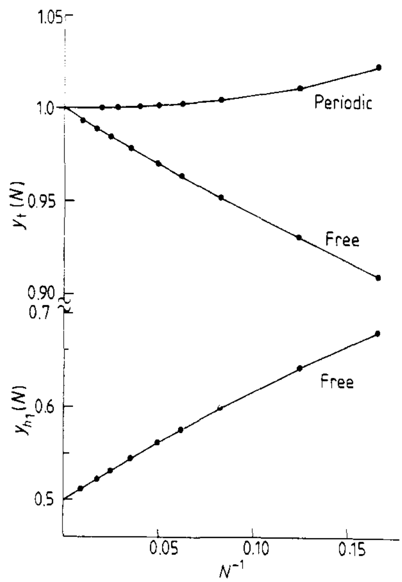

Figure 5. Estimates $y_t(N)$ and $y_{h_1}(N)$ of the exact scaling indices $y_t = 1$, $y_{h_1} = \frac{1}{2}$ obtained with phenomenological renormalisation. 'Free' and 'periodic' label results for strips of triangular lattice with free boundary conditions and strips of square lattice with periodic boundary conditions, respectively.

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