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LETTER TO THE EDITOR

Semi-infinite two-dimensional Ising model with marginally inhomogeneous couplings and conformal invariance

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Abstract. We consider a semi-infinite two-dimensional Ising model with nearest-neighbour couplings that deviate from the bulk critical coupling by Al^{-1}, where l is the distance from the surface. The surface critical exponents of this system are non-universal. Under a conformal mapping onto a strip of width L, the Al^{-1} inhomogeneity transforms into $A[(L/\pi)\sin(\pi l/L)]^{-1}$. For the square lattice the spectrum of the transfer matrix in the strip geometry is calculated exactly in the extreme anisotropic limit. The analytical results and numerical results for the triangular lattice are compared with predictions of conformal invariance.

The surface critical behaviour of semi-infinite magnetic systems with smoothly inhomogeneous coupling constants that deviate from the bulk critical coupling by Al^{-s} for large l, l being the distance from the boundary, is studied in [1-4]. According to scaling arguments [4] the inhomogeneity is irrelevant, marginal, and relevant for $s > y_t$, $s = y_t$, and $s < y_t$, respectively, where y_t is the bulk thermal scaling index. In the marginal case one expects non-universal surface critical behaviour, which is indeed found in the two-dimensional Ising model [1-3]. For $A < A_c$ (A_c being a positive constant) the correlation function of surface spins $g_{\|}(r)$ behaves asymptotically as $r^{-\eta_{\|}}$, where $\eta_{\|}(A) = 1 - A/A_c$. For $A > A_c$ there is a spontaneous surface magnetisation m_1, corresponding to $\eta_{\|} = 0$, and $g_{\|}(r) - m_1^2$ decays as $r^{-\eta_{\|}'}$, where $\eta_{\|}'(A) = -1 + A/A_c$.

In two-dimensional critical systems with homogeneous couplings conformal invariance determines all the bulk and surface critical exponents and correlation functions [5]. Conformal invariance also holds in systems where the translational invariance is broken by a marginally relevant defect line [6, 7]. In this letter we check the validity of conformal invariance in the semi-infinite two-dimensional Ising model with a marginal Al^{-1} inhomogeneity. Following a familiar recipe [8], we compare the exact correlation function of the system defined on a strip with the correlation function that follows from a conformal mapping of the half space onto the strip.

In spatially inhomogeneous systems the temperature variable $t(\boldsymbol{r})$ that specifies the local deviation from criticality transforms [4] as $t(\boldsymbol{r}') = b^{y_t} t(\boldsymbol{r})$ under an ordinary scaling transformation $\boldsymbol{r}' = b^{-1}\boldsymbol{r}$ and as

$$t(w) = |w'(z)|^{-y_t} t(z) \tag{1}$$

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under a conformal mapping $w = w(z)$. From the mapping $w = (L/\pi)\ln z$, with $z = x + iy$ and $w = u + iv$, one finds that $t(z) = Ay^{-s}$ in the half-space $y > 0$ corresponds to

$$t(w) = A(\pi/L)^{y_t} \exp[(y_t - s)\pi u/L][\sin(\pi v/L)]^{-s} \tag{2}$$

in the strip $0 < v < L$. In the marginally-inhomogeneous Ising model, $y_t = s = 1$ and

$$t(w) = A[(L/\pi)\sin(\pi v/L)]^{-1}. \tag{3}$$

Conformal covariance of the correlation function implies [8] the amplitude-exponent relation†

$$\lim_{L\to\infty} \frac{\xi_L(A)}{L} = \frac{2}{\pi\eta_\parallel(A)}. \tag{4}$$

Here $\eta_\parallel(A)$ is the non-universal exponent defined above, and $\xi_L(A)$ is the correlation length in the strip with inhomogeneous interactions of the form (3).

The surface scaling dimensions x_i of the operators can be determined from the spectrum of the transfer matrix T along the strip. We define the critical Hamiltonian H by $T = \exp(-aH)$, where a is the lattice spacing. Generally for free-spin boundary conditions H has a spectrum in the large-L limit of the form [5]

$$E_i - E_0 = \zeta\frac{\pi}{L}(x + m). \tag{5}$$

Here E_0 and E_i are the energies of the ground and ith excited states of H, respectively, and m is a non-negative integer. For classical two-dimensional systems with isotropic interactions, $\zeta = 1$, while for one-dimensional quantum models ζ is a normalising factor, the so-called sound velocity. In general $x_i = x + m$, where x is the anomalous dimension of a primary operator. The surface scaling index x_1^s of the magnetisation and the exponent $\eta_\parallel$ introduced above satisfy $\eta_\parallel = 2x_1^s$.

We have checked equation (4) numerically for the Ising model with a marginal inhomogeneity on the triangular lattice and calculated the complete spectrum of the transfer matrix for the square lattice analytically in the extreme anisotropic limit.

Our numerical studies consider [9] a semi-infinite triangular lattice with nearest-neighbour coupling constants $K_1(l)$ parallel to the surface and diagonal bonds $K_2(l)$ that vary as

$$K_j(l) = K_j(\infty) + A_j/l \tag{6a}$$

$$A_1 = \tfrac{1}{2}A\sinh(2K_1(\infty)) \qquad A_2 = \tfrac{1}{4}A\cosh(2K_2(\infty)). \tag{6b}$$

The bulk couplings $K_1(\infty) = K_2(\infty) = (\ln 3)/4$ are isotropic and critical. In the strip geometry A_j/l is replaced by $A_j[(L/\pi)\sin(\pi l/L)]^{-1}$, as in equation (3).

Using the numerical procedure outlined in [9] we have calculated the correlation length in strips of triangular lattice with widths of up to $N = 100$ triangles, i.e., $L = \sqrt{3}N/2$ lattice constants. The results are shown in figure 1. According to the amplitude-exponent relation (4), $2L/[\pi\xi_L(A)]$ should extrapolate to $\eta_\parallel(A) = 1 - A/A_c$

† Transformation (1) also leads to an amplitude-exponent relation for the two-dimensional Ising model with an interior defect line [6, 7]. Substituting $t(z) = B\delta(y)$ and $w = (L/2\pi)\ln z$ into equation (1), one obtains $t(w) = B[\delta(v) + \delta(v - L/2)]$ for $y_t = 1$. Conformal covariance of the correlation function implies $\lim_{L\to\infty}[\xi_L(B)/L] = [\pi\eta_\parallel(B)]^{-1}$. The non-universal exponent $\eta_\parallel(B)$ describes the decay of spin correlations parallel to the defect line, and $\xi_L(B)$ is the correlation length in a strip with two defect lines and cylindrical boundary conditions. This amplitude-exponent relation was first tested numerically in [6].

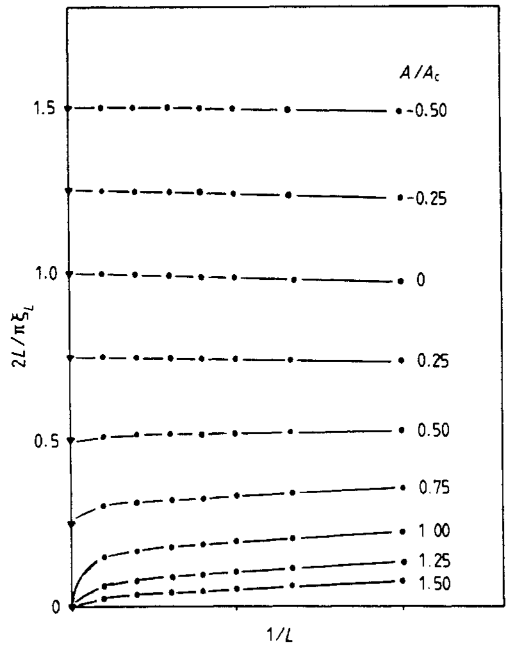

Figure 1. Numerical test of the amplitude-exponent relation (4) for strips of triangular lattice with width $L=\sqrt{3}N/2$ lattice constants and $N=10, 15, 20, 25, 33, 50, 100$. The triangles show the limiting values $\eta_{\parallel}(A)=1-A/A_c$ for $A<A_c$ and $\eta_{\parallel}(A)=0$ for $A>A_c$ predicted by (4).

for $A/A_c<1$ and to zero for $A/A_c>1$. These values are indicated by triangles on the figure. The agreement is very convincing for $A/A_c\leqslant 0.5$. For $A/A_c\geqslant 0.5$ the convergence with increasing L is slower, as explained quantitatively below, and the numerical results are less conclusive.

We now check equation (4) analytically and determine the scaling dimension of all the operators. We begin with a semi-infinite square lattice. As in [1] the couplings parallel to the surface are chosen to be position independent, i.e. $K_1(l)=K_1(\infty)$. The perpendicular bonds vary as

$$K_2(l)=K_2(\infty)+\tfrac{1}{4}A\sinh(2K_2(\infty))l^{-1} \qquad l\to\infty. \tag{7}$$

In the strip geometry the parallel couplings are again assumed to be position independent, while the perpendicular bonds have the spatial dependence (3). The critical Hamiltonian is determined in the extreme anisotropic or time-continuum limit [10]. This leads to a quantum Ising model with Hamiltonian

$$H=-\sum_{l=1}^{L-1}\lambda(l)\sigma_l^z\sigma_{l+1}^z-h\sum_{l=1}^{L}\sigma_l^x \tag{8a}$$

$$\lambda(l)=1-\alpha[(L/\pi)\sin(\pi l/L)]^{-1}. \tag{8b}$$

The σ_l^z, σ_l^x are Pauli operators at site l. The bulk critical point corresponds to $h=1$, and in the extreme anisotropic limit $A=-2\alpha$.

We calculate the spectrum of the critical Hamiltonian (8) to order $1/L$ following [11, 12]. The Hamiltonian is written as a quadratic expression in terms of fermion creation and annihilation operators and converted to the diagonal form

$$H=\sum_k\Lambda_k(a_k^+a_k-\tfrac{1}{2}) \tag{9}$$

by a canonical transformation. Here a_k, a_k^+ denote fermion operators and Λ_k the eigenvalues of an $L \times L$ matrix. As in [12] there is a systematic expansion in powers of $1/L$ for the lowest eigenvalues Λ_k, which are $O(1/L)$. To first order in $1/L$ the difference equation satisfied by the eigenvectors may be replaced by the differential equation

$$\phi''(x)+\left[\left(\frac{\Lambda L}{2\pi}\right)^2-\frac{\alpha^2+\alpha\cos x}{\sin^2 x}\right]\phi(x)=0 \tag{10}$$

with boundary conditions

$$\phi(x)|_{x=0}=0 \qquad \left(\frac{\alpha}{\sin x}\phi(x)+\phi'(x)\right)\bigg|_{x=\pi}=0. \tag{11}$$

Here $0 \leqslant x=\pi l/L \leqslant \pi$, and in equation (10) we have omitted the index k. One sees in (10) that Λ is $O(1/L)$ as originally assumed.

With the substitutions

$$\phi(x)=\cos^{\alpha}(x/2)\sin^{\alpha+1}(x/2)y(t) \qquad t=\sin^2(x/2) \tag{12}$$

equation (10) can be rewritten in the hypergeometric form [13]

$$t(1-t)y''(t)+[c-(a+b+1)t]y'(t)-aby(t)=0 \tag{13a}$$

$$a=\alpha+1/2+\Lambda L/2\pi \qquad b=\alpha+1/2-\Lambda L/2\pi \qquad c=\alpha+3/2. \tag{13b}$$

The general solution to equation (13) is given by

$$y(t)=C_1F(a,b;c;t)+C_2t^{1-c}F(a-c+1,b-c+1;2-c;t) \tag{14}$$

where the $F(a,b;c;t)$ are standard hypergeometric functions [13]. The boundary condition (11) at $x=0$ requires $C_2=0$ for $\alpha>-\frac{1}{2}$ and $C_1=0$ for $\alpha<-\frac{1}{2}$. Both boundary conditions (11) are only satisfied for the discrete set of eigenvalues†

$$\Lambda_k=\frac{2\pi}{L}(\alpha+\tfrac{1}{2}+k) \qquad k=0,1,2,\ldots \quad \alpha>-\tfrac{1}{2} \tag{15a}$$

$$\Lambda_0=O(L^{2\alpha}) \qquad \Lambda_k=\frac{2\pi}{L}(-\alpha+\tfrac{1}{2}+k-1) \qquad k=1,2,3,\ldots \quad \alpha<-\tfrac{1}{2}, \tag{15b}$$

corresponding to hypergeometric functions that are finite polynomials.

The α dependence of the first few eigenvalues is shown in figure 2. For $\alpha<-\frac{1}{2}$ the lowest eigenvalue $\Lambda_0 \sim L^{2\alpha}$ vanishes faster than L^{-1} in the large-L limit. Thus the ground state of the system is asymptotically degenerate, i.e., there is a spontaneous surface magnetisation in the limit $L\to\infty$, in accordance with previous results [1-3].

The spontaneous surface magnetisation for $\lambda(\infty)\geqslant 1$, $\alpha<-\frac{1}{2}$ disappears discontinuously [1-4] as $\lambda(\infty)$ is lowered past 1. In a first-order transition the correlation length ordinarily remains finite, and in the large-L limit the gap in the spectrum of the transfer matrix varies [14, 15] as $\exp(-\sigma L)$ at and below the transition temperature. However, in the first-order transition in our system the correlation length diverges, and the gap vanishes according to a power law in L instead of exponentially.

† Equations (10) and (11), which only determine Λ to order L^{-1}, yield $\Lambda_0=0$ for $\alpha<-\frac{1}{2}$. The result $\Lambda_0 \sim L^{2\alpha}$ can be derived from the difference equation for eigenvectors, using the continuum eigenfunction $\phi(x)=\tan^{-\alpha}(\pi l/2L)$ as a first approximation.

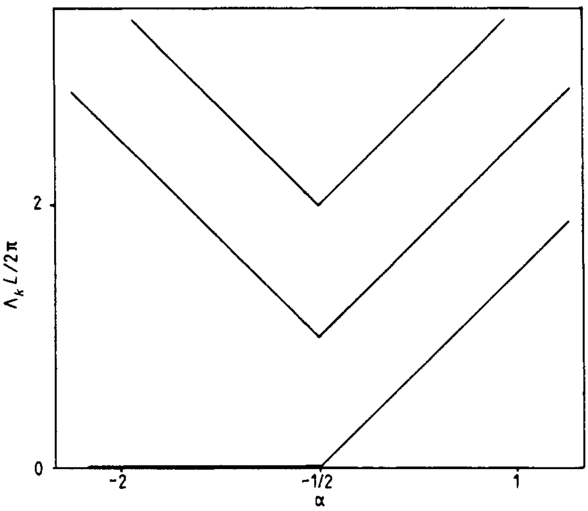

Figure 2. Dependence of the lowest few eigenvalues Λ given by equation (15) on α.

Now we determine the anomalous dimensions of the scaling operators from equations (5), (9), and (15). The value $\zeta = 2$ for the second velocity follows from earlier work [16] on the homogeneous model ($\alpha = 0$). The excited states of H belong to orthogonal sectors containing odd (magnetisation sector) and even (energy sector) numbers of fermions, respectively.

For $\alpha > -\frac{1}{2}$, corresponding to zero surface magnetisation, the anomalous dimensions in the magnetisation sector are given by

$$x_i^s = n + \tfrac{1}{2} + (2m+1)\alpha \qquad n, m = 0, 1, \ldots \tag{16}$$

The least dimension $x_1^s = \frac{1}{2} + \alpha$ in this sector coincides with the value $\eta_\parallel/2$ deduced from the pair correlation function in the semi-infinite geometry [1-3]. Thus the amplitude-exponent relation (4) is satisfied.

In the energy sector one finds the anomalous dimensions

$$x_i^e = n + 2m\alpha \qquad n = 2, 3, \ldots \quad m = 1, 2, \ldots \tag{17}$$

The least scaling dimension $x_1^e = 2 + 2\alpha$, which describes the decay of surface energy correlations, is consistent with numerical results for the semi-infinite geometry [17]. In both sectors there are conformal towers of the form (5). The number of primary operators is finite (q) if α is a rational number ($\alpha = p/q$ where p, q are relative primes) and is infinite if α is irrational.

For $\alpha < -\frac{1}{2}$, corresponding to a non-vanishing surface magnetisation, the critical dimensions are given by formulae similar to (16) and (17), except that α is replaced by $-\alpha$. Again the spectrum has the form (5), but the scaling dimension $x' = \eta'_\parallel/2 = -\frac{1}{2} - \alpha$ deduced from the result for $\eta'_\parallel$ in the semi-infinite geometry [1-3] is absent.

According to equation (1), $t(z) = Ay^{-y_t}$ is invariant under Möbius mappings of the half space $y > 0$ onto itself. Thus conformal invariance implies the functional form [5, 18]

$$g(x_1 - x_2; y_1, y_2) = (y_1 y_2)^{-\eta/2} F\{y_1 y_2/[(x_1 - x_2)^2 + (y_1 - y_2)^2]\} \tag{18}$$

for the spin-spin correlation function, where $\eta = \frac{1}{4}$ for the Ising model. The exact results reviewed in the first paragraph of this letter are reproduced if $F(u) \approx Bu^{\eta_\parallel/2}$

for $A < A_c$ and $F(u) \approx C^2 + Du^{\eta_\parallel'/2}$ for $A > A_c$ as $u \to 0$. However, from other arguments it seems that the amplitudes C^2 and D must vanish. If (18) applied with D non-zero, the scaling dimension $x' = \eta_\parallel'/2$ would be present in the spectrum of the transfer matrix, which is not the case. C must vanish since an $L \times \infty$ Ising strip with finite couplings has zero spontaneous magnetisation except at $T = 0$. If C were non-zero, the half-space magnetisation $m(y) = Cy^{-1/8}$ would transform into a non-zero spontaneous magnetisation in the strip under the logarithmic mapping [19]. Presumably $F(u)$ vanishes identically for $A > A_c$, and the exact results of the first paragraph represent corrections to (18). As a check on this interpretation, it would be nice to have exact results for the magnetisation profile at T_c in the inhomogeneous semi-infinite Ising model with $A > A_c$ to see whether $m(y)$ does indeed decay faster than $y^{-1/8}$ perpendicular to the boundary.

We have checked our analytical results for the spectrum in detail by diagonalising the Hamiltonian (8) numerically for chain lengths up to $L = 200$. For the triangular lattice we have also numerically confirmed the analogue $\xi_L^{-1} \sim L^{-A/A_c}$, $A > A_c$ (see figure 1) of the relation $\Lambda_0 \sim L^{2\alpha}$, $\alpha < -\frac{1}{2}$.

The algebra that generates the spectrum of the transfer matrix will be constructed explicitly in a subsequent publication [20].

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